

Spreading Processes on Networks: Models, Techniques and Algorithms

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"numerical techniques for social media and network problems"

- "computational social science":
 - large-scale data is being collected on complex social systems
 - online social networks (Facebook, Twitter, ...)
 - email (gmail, ...)
 - travel patterns (public transportation, google maps, ...)
 - mobile phone connections, locations
 - shopping patterns
 - ...
 - it is now possible to build, analyze, and simulate computational models of these systems.
 - research is possible that <u>applies successful methods from the natural sciences</u>, e.g. mathematical modelling and statistical mechanics, to produce novel insights in the social sciences apply 'scientific method '' to social science
 - some of this can be high-performance computing / high-end computing (big data, combinatorial, ...), efficient algorithms, methods



"numerical techniques for social media and network problems"

- I have started to set some steps in computational social science / network problems / social media (numerical PDEs, numerical linear algebra, numerical optimization, HPC)
 - multigrid methods for computing stationary vectors of Markov chains random walks on graphs (Google PageRank) → Nelly Litvak
 - multilevel co-clustering for social networks
 - location tagging for Twitter messages
 - optimization methods for tensor decomposition, matrix completion, recommendation
 - ODE and network models for social uprisings (Arab Spring)
 - dynamical models for smoking epidemic and obesity epidemic
 - propagation of Susceptible-Infectious-Recovered (SIR) disease on random networks with spatial structure



"numerical techniques for social media and network problems"

"propagation of Susceptible-Infectious-Recovered (SIR) disease on random networks with spatial structure"

- "introduction to network science"
- some new results on SIR propagation on random spatial networks
- Spreading Processes on Networks:
 - Models
 - Techniques
 - Algorithms (random network generation, stochastic simulation algorithms)
 - Applications

Random Spatial Networks: Small Worlds without Clustering, Traveling Waves, and Hop-and-Spread Disease Dynamics

John Lang, Hans De Sterck, Jamieson L. Kaiser, Joel C. Miller



arXiv:1702.01252v1

collaborators

Joel Miller, Institute for Disease Modeling, Seattle, USA



John Lang, UCLA, Communications Studies (PhD Waterloo, July 2016)





sources (background on network science, SIR disease propagation, ...)

http://barabasi.com/networksciencebook/ **NETWORK SCIENCE CLASS 3: RANDOM NETWORKS** (CHAPTER 3 IN TEXTBOOK) Albert-László Barabási with Roberta Sinatra WWW.BARABASILAB.COM

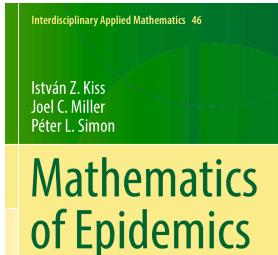
arXiv:1702.01252v1



Random Spatial Networks: Small Worlds without Clustering, Traveling Waves, and Hop-and-Spread Disease Dynamics

John Lang, Hans De Sterck, Jamieson L. Kaiser, Joel C. Miller

book by Kiss, Miller and Simon (2017)



on Networks

From Exact to Approximate Models



motivation: spread of 2013-2016 Ebola epidemic

• Guinea, Sierra Leone, Liberia

Virus genomes reveal factors that spread and sustained the Ebola epidemic

Gytis Dudas, Luiz Max Carvalho, Trevor Bedford, Andrew J. Tatem, Guy Baele, *Nature* **544**, 309–315 (20 April 2017) | doi:10.1038/nature22040

- goal: develop modeling framework
- random networks
- spatial structure!
- disease propagation (stochastic, DEs for insight)



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two parts of my presentation

- part A: models and algorithms for networks
 - "introduction to network science"
 - random spatial networks
 - algorithms for efficient network generation
 - application: small worlds with spatial structure
- part B: disease propagation on networks
 - propagation of Susceptible-Infectious-Recovered (SIR) disease
 - stochastic simulation algorithms
 - exact analytic models, and simulations
 - applications

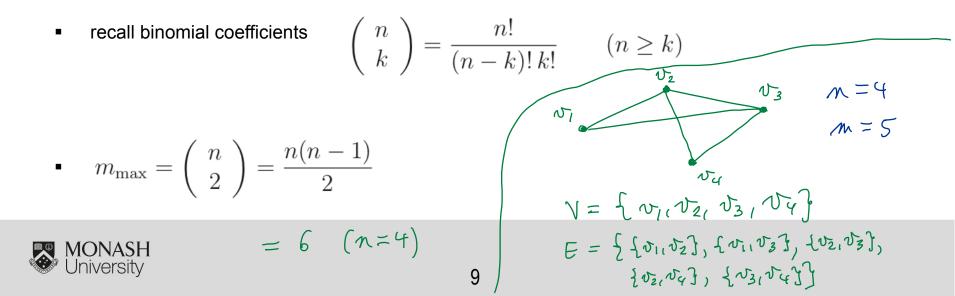


A1: a brief overview of graphs and networks

• graph G = (V, E) (undirected, simple (no loops, no multiple edges))

- vertices/nodes
$$V = \{v_1, v_2, \dots, v_n\}$$
 $n = |V|$

- edges
$$E = \{\{v_{i_1}, v_{j_1}\}, \dots, \{v_{i_m}, v_{j_m}\}\}$$
 $m = |E|$



nodal degrees

• degree k_i = number of edges incident on node v_i

• average degree
$$< k > = \frac{\sum_{i=1}^{n} k_i}{n}$$

$$y: \qquad \sum_{i=1}^{n} k_i = 2m$$

$$m = \frac{n < k >}{2}$$

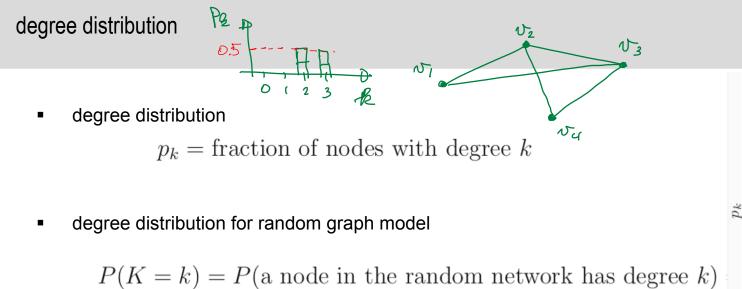
$$B_2 = 3$$

 $R_1 = 2$

L Q> = 2.5

 $5 = \frac{4 \cdot 2.5}{2}$

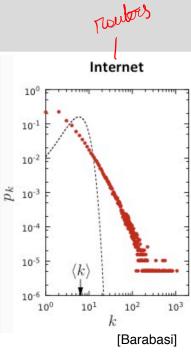




many "real-world" networks approximately have power law degree distribution

$$p_k = ck^{-\gamma} \qquad 2 \le \gamma \le 3$$





counting triangles - clustering coefficient

local clustering coefficient of node v_i

Nu $c_i = \frac{\text{\# of triangles node } v_i \text{ forms with its neighbors}}{\text{\# of possible triangles node } v_i \text{ can form with its neighbors}}$ $c_{i} = \frac{1}{\#} \text{ of possible under }$ neighbor set of node $\frac{v_{i}}{v_{i}}$ $N_{i} = \{v_{i_{1}}, \dots, v_{i_{k_{i}}}\}$ $E_{N_{i}} = \{\text{edges between neighbors of node } v_{i}\}$ $C_{i} = \frac{1 + 1 + \frac{2}{3} + \frac{2}{3}}{2|E_{N_{i}}|}$ $E_{N_{i}} = \frac{1}{2} = \frac{1}{5}$ $C_2 = \frac{2}{3}$ $C_1 = \frac{1}{1}$ then 15average clustering coefficient $\langle c \rangle = \frac{\sum_{i=1}^{n} c_i}{\sum_{i=1}^{n} c_i}$

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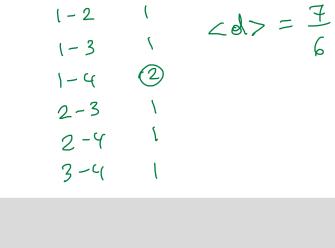
average shortest path

• $d_{ij} = \#$ of edges between nodes v_i and v_j , in a shortest path

average (shortest) path length (in a connected graph)

 $\langle d \rangle = \frac{\sum_{i>j} d_{ij}}{n(n-1)/2}$

- many "real-world networks" have
 - large clustering < c >:
 - small average path length $\ < d >$



 v_2

Nu

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V-3



example: Watts-Strogatz "small world" networks

Collective dynamics of 'small-world' networks

Duncan J. Watts* & Steven H. Strogatz

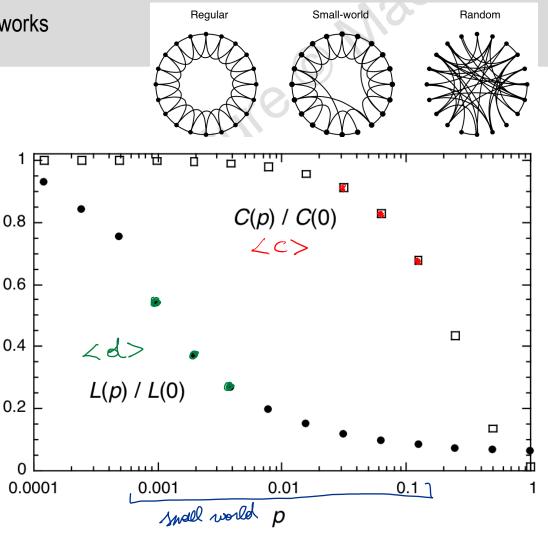
ring, each node connected to four nearest neighbors; randomly rewire with probability p (Nature) (1998) Small-world Random Regular (34,000) p=0p=1Increasing randomness



example: Watts-Strogatz "small world" networks

- small world:
 - high clustering <
 (local structure) (unlike random graph)
 - small average (shortest) path length $\angle \diamond >$
 - (good connectivity) (like random graph)
 - (16 degrees of separation " many "real world" graphs are
- many "real-world" graphs are small-world

"lærge world": (e.g., lættice) - lærge (average) stortest pælt length $\frac{\text{MONASH}}{\text{University}} \quad \angle d > = O(n)$ 1D lettice

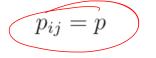


A2: some random network models

Erdos-Renyi networks. n nodes, and assign edges randomly with probability p

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 $p_{ij} = P(\text{edge } \{v_i, v_j\} \text{ exists})$

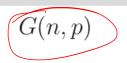


- degrees and edges:
 - $k_i \approx (n-1)p$

$$E(k_i) = (n-1)p$$

$$E(\langle k \rangle) = (n-1)p$$





 $E(m) = \frac{n(n-1)}{2}p$

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Erdos-Renyi networks: degree distribution

binomial degree distribution

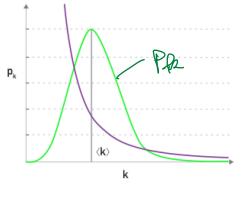
$$p_k = P(K = k) = \binom{n-1}{k} p^k (1-p)^{(n-1)-k}$$

$$E(k) = (n-1)p$$
 $Var(k) = \sigma^{2}(k) = p(1-p)(n-1)$

peaked distribution!

$$\frac{\sigma(k)}{E(k)} = O\left(\frac{1}{\sqrt{n-1}}\right)$$

No



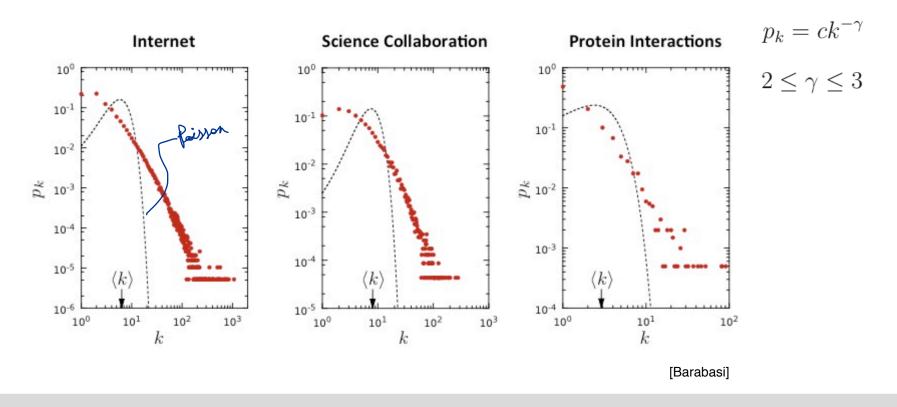
[Barabasi]

for large n, small k: approximately Poisson distributed

$$p_k \approx \exp(-\lambda) \frac{\lambda^k}{k!} \qquad E(k) = \lambda \qquad \lambda = (n-1)p$$



degree distributions of "real" networks: power law graphs - scale-free networks





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"real world" networks with power law distribution (approximately)

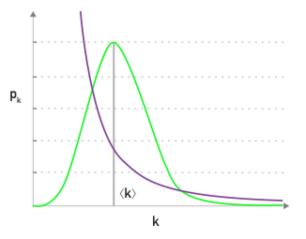
	Network	Ν	L	(k)	$\langle k_{in}^2 \rangle$	⟨k _{out} ²⟩	(k ²)	Yin	Yout	Y
tef	Internet	192,244	609,066	6.34	-	-	240.1	-	-	3.42*
	www	325,729	1,497,134	4.60	1546.0	482.4	-	2.00	2.31	-
	Power Grid	4,941	6,594	2.67	-	-	10.3	-	-	Exp.
Social	Mobile-Phone Calls	36,595	91,826	2.51	12.0	11.7	-	4.69*	5.01*	-
	Email	57,194	103,731	1.81	94.7	1163.9	-	3.43*	2.03*	-
	Science Collaboration	23,133	93,437	8.08	-	-	178.2	-	-	3.35*
	Actor Network	702,388	29,397,908	83.71	-	-	47,353.7	-	-	2.12*
	Citation Network	449,673	4,689,479	10.43	971.5	198.8	-	3.03*	4.00*	-
ltio	E. Coli Metabolism	1,039	5,802	5.58	535.7	396.7	-	2.43*	2.90*	-
	Protein Interactions	2,018	2,930	2.90	-	-	32.3	-	-	2.89*-

Table 4.1



[Barabasi]

degree distributions of "real" networks: power law graphs - scale-free networks



Random Network Randomly chosen node: $k = \langle k \rangle \pm \langle k \rangle^{1/2}$ Scale: $\langle k \rangle$

Scale-Free Network

Randomly chosen node: $k = \langle k \rangle \pm \infty$ Scale: none

[Barabasi]

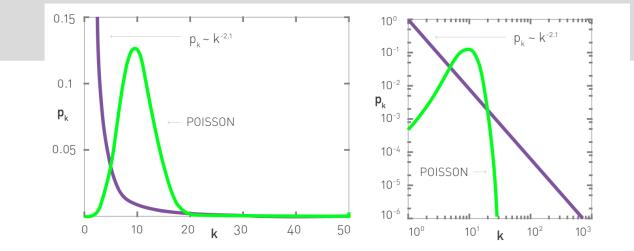


$$p_k = ck^{-\gamma} \qquad 2 \le \gamma \le 3$$

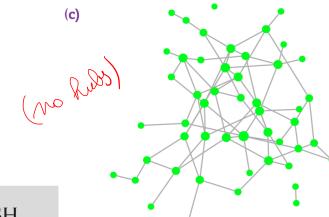
$$E(k^l)$$
 $l > \gamma - 1$ diverges

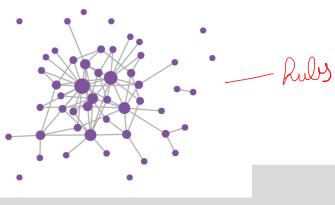
$$\gamma < 3: l = 2, 3, \dots$$
 diverge

 $E(k^2)$ diverges



(d)

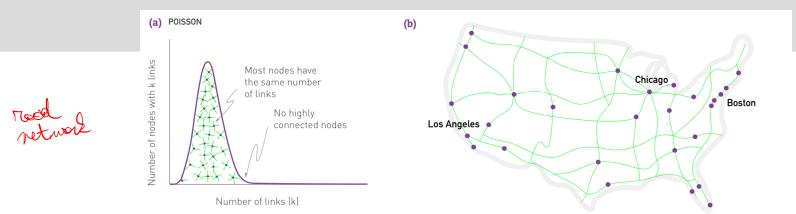




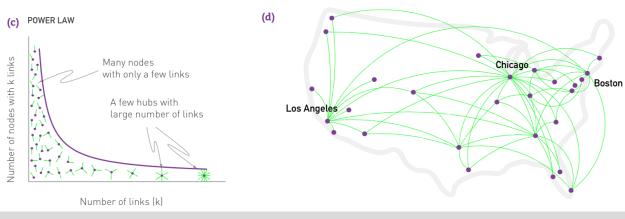


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[Barabasi]







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[Barabasi]

Erdos-Renyi networks: average shortest path

small-world network!

> $d_{ii} = \#$ of edges between nodes v_i and v_i , in a shortest path $E(d) \approx \frac{\log(n)}{\log(E(k))} \qquad \text{ overage skriftst path: } E(d) = O(\log(n)),$

- compare
 - 1D lattice: E(d) = O(n)- 2D lattice; $E(d) = O(\sqrt{n})$





"real-world" networks: average shortest path

small worlds!

 $E(d) \approx \frac{\log(n)}{\log(E(k))}$ Endes - Penyi

shortest path						dianoter		
Network	N	L	‹k› ((d)	d _{max}	lnN/ln <k></k>		
Internet	192,244	609,066	6.34	6.98	26	6.58		
www	325,729	1,497,134	4.60	11.27	93	8.31		
Power Grid	4,941	6,594	2.67	18.99	46	8.66		
Mobile-Phone Calls	36,595	91,826	2.51	11.72	39	11.42		
Email	57,194	103,731	1.81	5.88	18	18.4		
Science Collaboration	23,133	93,437	8.08	5.35	15	4.81		
Actor Network	702,388	29,397,908	83.71	3.91	14	3.04		
Citation Network	449,673	4,707,958	10.43	11.21	42	5.55		
E. Coli Metabolism	1,039	5,802	5.58	2.98	8	4.04		
Protein Interactions	2,018	2,930	2.90	5.61	14	7.14		
Table a c				\smile				

Table 3.2

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Erdos-Renyi networks: clustering coefficient

$$c_{i} = \frac{2|E_{N_{i}}|}{k_{i}(k_{i}-1)} \approx p = \frac{E(k)}{n-1}$$
connected neighbor pairs
total neighbor pairs

- low clustering as n grows
- but: many "real-world" networks have high average clustering coefficients

Network	C	Erdös-Rényi	Î
Web [2]	0.081	7.71	
Flickr	0.313	47,200	
LiveJournal	0.330	119,000	
Orkut	0.171	7,240	
YouTube	0.136	36,900	(A. Bonato)



random networks with more realistic degree distributions: Chung-Lu networks

- n nodes, desired degree sequence $\{\kappa_1, \ldots, \kappa_n\}$
- add edges randomly according to

$$p_{ij} = P(\text{edge } \{v_i, v_j\} \text{ exists})$$

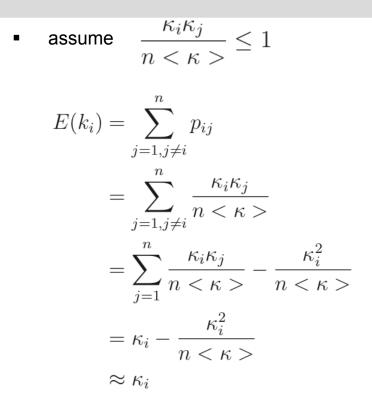
$$\left(p_{ij} = \frac{\kappa_i \kappa_j}{n < \kappa >}\right) \qquad <\kappa > = \frac{\sum_{i=1}^n \kappa_i}{n}$$

$$p_{ij} = \max(\frac{\kappa_i \kappa_j}{n < \kappa >}, 1)$$

(advantage: edges assigned independently, which keeps the model "analyzable" ... see later)



Chung-Lu networks: expected degree



- Chung-Lu as a model for "realworld" networks:
 - path length < d > OK!
 - degree distribution p_k OK!
 - clustering coefficient < c > too low ...



Chung-Lu networks: choose desired degrees from distribution

• note: desired degree sequence $\{\kappa_1, \ldots, \kappa_n\}$ can be chosen from (continuous) distribution

 $p(\kappa)$

$$E(\kappa) = \int_0^\infty \kappa p(\kappa) d\kappa \qquad \qquad p_{ij} = \frac{\kappa_i \kappa_j}{n < \kappa >}$$

$$E(k_i) = \int_0^\infty \frac{\kappa_i \kappa}{n \int_0^\infty \kappa p(\kappa) d\kappa} n p(\kappa) d\kappa = \kappa_i$$

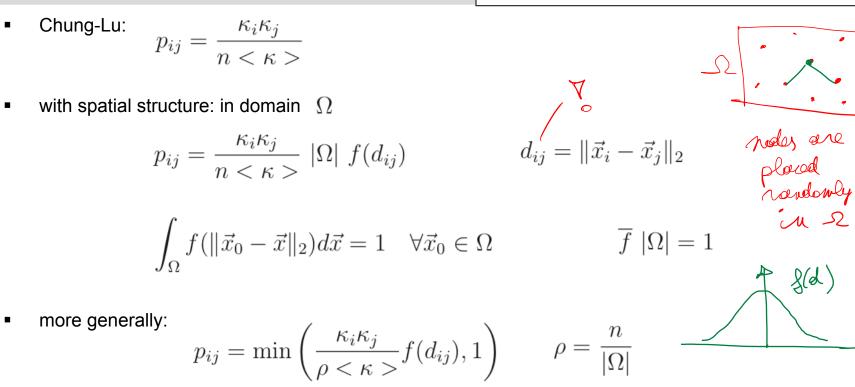
$$\int_0^\infty \int_0^\infty \kappa p(\kappa) d\kappa = \kappa_i$$
is expected degree is \mathcal{K}_i .



A3: random spatial networks (RSNs)

Random Spatial Networks: Small Worlds without Clustering, Traveling Waves, and Hop-and-Spread Disease Dynamics

John Lang, Hans De Sterck, Jamieson L. Kaiser, Joel C. Miller





random spatial networks (RSNs)

$$p_{ij} = \min\left(\frac{\kappa_i \kappa_j}{\rho < \kappa >} f(d_{ij}), 1\right)$$
portion of network
observed degrees
observed edge lengths
observed edge lengths

FIG. 1. An example RSN and its properties. The distance kernel is a Gaussian, $f(d) = \exp(-d^2/2\sigma^2)/2\pi\sigma^2$ with $\sigma = 0.03$. The imposed distribution of expected degrees is P(2) = P(15) = 0.5. The density is $\rho = 10000$. One node and its neighbors are highlighted. A random network without spatial structure would exhibit neighbors throughout the domain.



random spatial networks (RSNs): expected degree

$$p_{ij} = \min\left(\frac{\kappa_i \kappa_j}{\rho < \kappa >} f(d_{ij}), 1\right)$$

$$E(k_i) = \int_{\kappa=0}^{\infty} \left(\int_{\Omega} \frac{\kappa_i \kappa}{\rho \int_0^{\infty} \kappa p(\kappa) d\kappa} f(\|\vec{x}_i - \vec{x}\|_2) \rho d\vec{x}\right) p(\kappa) d\kappa$$

$$= \kappa_i \frac{\int_0^{\infty} \kappa p(\kappa) d\kappa}{\int_0^{\infty} \kappa p(\kappa) d\kappa} \int_{\Omega} f(\|\vec{x}_i - \vec{x}\|_2) d\vec{x}$$

$$= \kappa_i$$



A4: efficient algorithms for network generation

• Erdos-Renyi:
$$G(n, p)$$

 $p_{ij} = p$

- naive algorithm
 - for each possible edge $\{v_i, v_j\}$, draw a random number

$$m_{\max} = \left(\begin{array}{c} n\\2 \end{array}\right) = \frac{n(n-1)}{2}$$

– complexity
$$O(n^2)$$



efficient algorithms for network generation

Efficient Generation of Large Random Networks*

Vladimir Batagelj[†] Department of Mathematics, University of Ljubljana, Slovenia.

- Ulrik Brandes[‡] Department of Computer & Information Science, University of Konstanz, Germany.
- Erdos-Renyi: O(n+m) algorithm $p_{ij} = p$
 - naive algorithm has many failures (when p is small)
 - idea: we know the distribution of successes and failures! (geometric); so sample the number of failures according to the appropriate distribution

 δ = number of failures before success

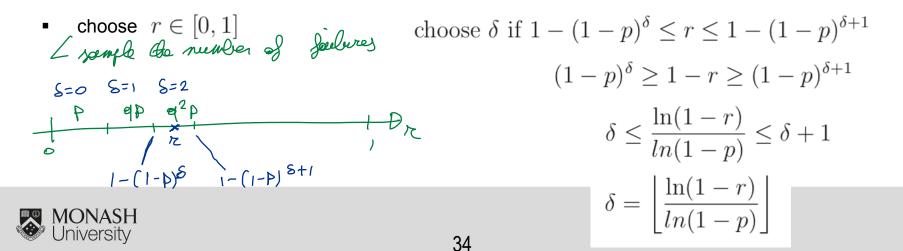
$$\begin{split} P(\delta) &= P(\text{first success happens at trial } \delta + 1) \qquad \delta = 0, 1, 2, \dots \\ &= (1-p)^{\delta} p \\ P(D \leq \delta) = P(\text{first success happens in trial } 1, 2, \dots, \text{ or } \delta + 1) \\ &= 1 - P(\text{no success in first } \delta + 1 \text{ trials}) \\ &= 1 - (1-p)^{\delta+1} \end{split}$$



efficient algorithms for network generation

• Erdos-Renyi: O(n+m) algorithm $p_{ij} = p$ q = 1 - p

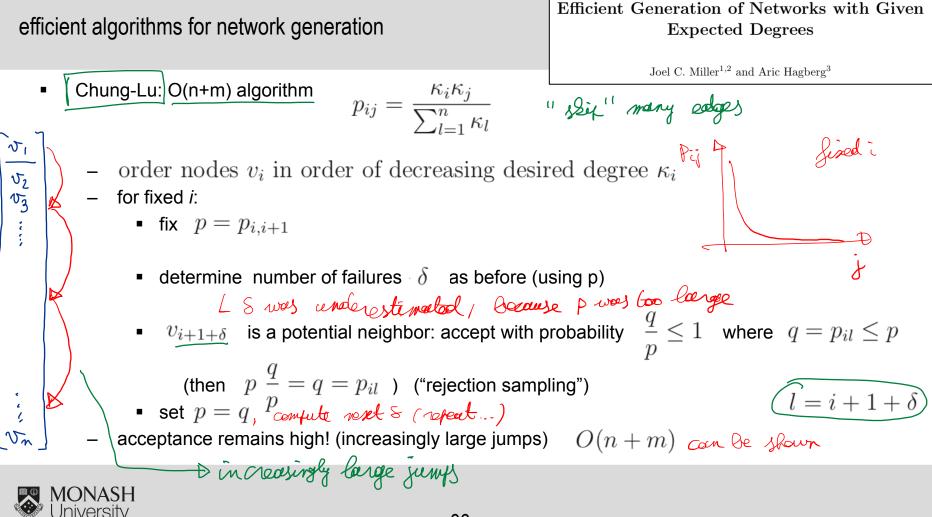
 $\delta = \text{ number of failures before success}$ $P(D \le \delta) = P(\text{first success happens in trial } 1, 2, \dots, \text{ or } \delta + 1)$ $= 1 - P(\text{no success in first } \delta + 1 \text{ trials})$ $= 1 - (1 - p)^{\delta + 1}$



Algorithm 1. G(N, p) Graph **Input:** number of nodes N, and probability 0**Output:** G(N, p) graph G(V, E) with $V = \{0, ..., N - 1\}$ $E \leftarrow \emptyset$ for u = 0 to N - 2 do $v \leftarrow u + 1$ Erner loop while v < N do choose $r \in (0, 1)$ uniformly at random N-1 $v \leftarrow v + \left\lfloor \frac{\log(r)}{\log(1-p)} \right\rfloor$ if v < N then $\begin{array}{cccc} E \leftarrow E \cup \{u, v\} & \longrightarrow & \text{m successes} \\ v \leftarrow v + 1 & & \text{fool} \end{array}$

$$O(n+m)$$
 (random numbers,



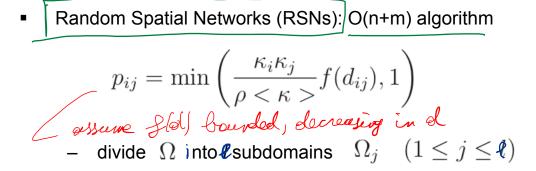


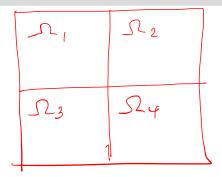
Algorithm 2. Chung-Lu Graph

```
Input: list of N weights, W = w_0, \ldots, w_{N-1}, sorted in decreasing order
Output: Chung-Lu graph G(V, E) with V = \{0, \dots, N-1\}
  E \leftarrow \emptyset
  S \leftarrow \sum_{u} w_u
  for u = 0 to N - 2 do
     v \leftarrow u + 1
     p \leftarrow \min(w_u w_v / S, 1)
      while v < N and p > 0 do
                                                                  - S P=1: S=0 (nothing
         if p \neq 1 then
            choose r \in (0, 1) uniformly at random
           v \leftarrow v + \left\lfloor \frac{\log(r)}{\log(1-p)} \right\rfloor
         if v < N then
            q \leftarrow \min(w_u w_v / S, 1)
            choose r \in (0, 1) uniformly at random
            if r < q/p then
                                                    O (n & m) can be shown
( acceptance is Best high)
               E \leftarrow E \cup \{u, v\}
            p \leftarrow q
            v \leftarrow v + 1
```



efficient algorithms for network generation





- order nodes in each subdomain by decreasing desired degree

$$p = \frac{\kappa_i \kappa_j}{\rho < \kappa >} f_{\max}$$

determine number of failures δ as before (using p)

choose Jman such that acceptance is leaft high (beep p close to the real PEJ)



efficient algorithms for network generation

Random Spatial Networks (RSNs): O(n+m) algorithm

$$p = \frac{\kappa_i \kappa_j}{\rho < \kappa >} f_{\max} - \theta \quad \text{mode sure } p \ge \Pr_{ij}$$

determine number of failures δ as before (using p) node u in region Ω_1

» edges within region 1:

$$f_{\max} = f(0)$$

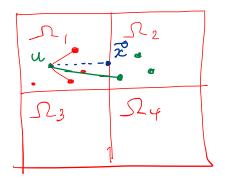
» edges to region Ω_2

find point \vec{x} in Ω_2 nearest to node u in region Ω_1 $f_{\max} = f(\|\vec{x} - \vec{x}_u\|_2) \xrightarrow{\bullet} \underbrace{\text{Brane is closen Swall, but}}_{\text{Legel exceptance}} \stackrel{\text{p} \geq \stackrel{\text{p}}{_{ij}} \stackrel{\text{remains high! (increasingly large jumps)}}_{O(n+m)}$

- acceptance remains high! (increasingly large jumps)

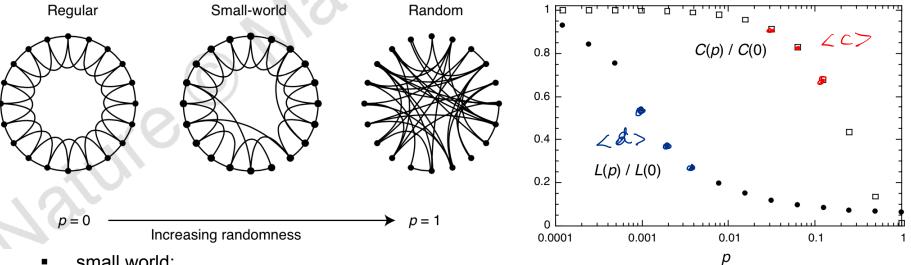


$$p_{ij} = \min\left(\frac{\kappa_i \kappa_j}{\rho < \kappa >} f(d_{ij}), 1\right)$$



A5: small world networks with spatial structure (RSNs)

recall: Watts-Strogatz "small world" networks



- small world:
 - large average local clustering coefficient —
 - $\langle d \rangle$ small average (shortest) path length _



<c>

small world networks with spatial structure (RSNs)

• RSNs: define local proximity coefficient

- first normalize all distances: \overline{d}_{ij} normalized to [0, 1]

- define local proximity coefficient:

 $p_i = 1 - \operatorname{avg}(\overline{d}_{ij} \text{ of graph neighbors } j \text{ of } i)$ $p_i \in [0, 1]$ $p_i \approx 1$: graph neighbors of i are located close $p_i \approx 0$: graph neighbors of i are located far

average local proximity coefficient:



small worlds with spatial structure

Jniversity

a specific class of RSNs: mostly local connections, few global connections

$$\kappa_{i} = k \qquad |\Omega = 1| \qquad \text{choose} \quad r_{0}$$

$$p_{ij} = \min\left(\underbrace{\kappa_{i}\kappa_{j}}{\rho < \kappa >} f(d_{ij}), 1\right)$$

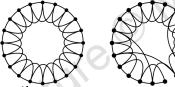
compute
$$N_0 = \frac{k}{\pi r_0^2}$$

 $p_{uv} = \min\left(k\frac{f(d_{uv})}{N}, 1\right) = \frac{kf(d_{uv})}{N}$

$$f(d_{uv}) = \begin{cases} \frac{N_0}{k} \left[1 - \epsilon \frac{1 - \pi r_0^2}{\pi r_0^2} \right] & d_{uv} < r_0 \\ \frac{N_0}{k} \epsilon & d_{uv} \ge r_0 \end{cases}$$

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$$g(d) = \frac{1}{r_0} \frac{1}$$



small worlds with spatial structure

a specific class of RSNs: mostly local connections, few global connections

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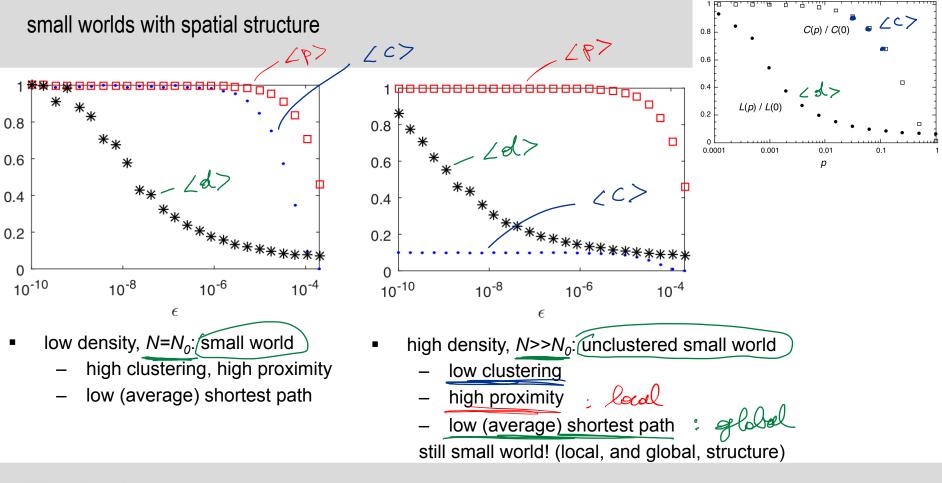
$$N_0 = \frac{k}{\pi r_0^2}$$

$$- case \ n = N_0, \ \epsilon \neq 0 \ : \text{ some long-range connections}}$$

$$N_0 = \frac{k}{\pi r_0^2}$$

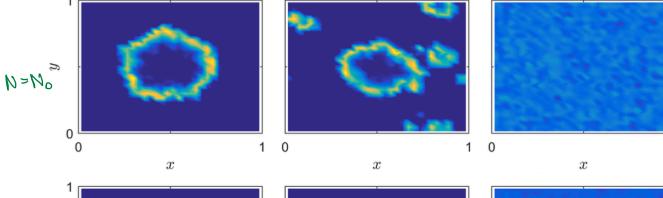
$$N_0 = \frac{k}{\pi r_0^2}$$

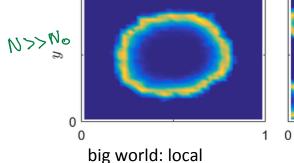
- case $n = N \gg N_0, \ \epsilon \neq 0$ < c >= O(1/N)
 - low density, low clustering, but proximity remains the same





$$\epsilon = 10^{-10} \qquad \epsilon = 10^{-7.25} \qquad \epsilon = \pi r_0^2$$





propagation

, ,

small world: local and

global propagation

0 uniform world: only small-world effect:

- local propagation (traveling wave) due to local structure (proximity, not clustering)
- long-range jumps due to small-world property

for spatial networks, proximity is important in determining whether small-world effects occur, rather than clustering





global propagation (no local structure)