Frontiers of Network Science Fall 2023

Class 3: Graph Theory & Random Networks (Chapter 2-3 in Textbook)

Boleslaw Szymanski

based on slides by Albert-László Barabási & Roberta Sinatra



UNDIRECTED VS. DIRECTED NETWORKS

Undirected

Links: undirected (symmetrical)

Graph:



Undirected links : coauthorship links Actor network protein interactions

Directed

Links: directed (arcs).

Digraph = directed graph:



An undirected link is the superposition of two opposite directed links.

Directed links : URLs on the www phone calls metabolic reactions

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NETWORK

Internet WWW Power Grid Mobile Phone Calls Email Science Collaboration Actor Network

Citation Network

E. Coli Metabolism

Protein Interactions

Routers Webpages Power plants, transformers Subscribers Email addresses Scientists Actors Paper Metabolites Proteins

NODES

LINKS Internet connections Links Cables Calls Emails Co-authorship Co-acting Citations Chemical reactions Binding interactions

Ν DIRECTED UNDIRECTED Undirected 609,066 192,244 Directed 325,729 1,497,134 Undirected 6,594 4,941 Directed 91,826 36,595 Directed 103,731 57,194 Undirected 93,439 23,133 Undirected 702,388 29,397,908 Directed 4,689,479 449,673 Directed 5,802 1,039 Undirected 2,018 2,930

Degree, Average Degree and Degree Distribution

BRIEF STATISTICS REVIEW

Four key quantities characterize a sample of N values $x_1, ..., x_N$:

Average (mean):

$$\langle x \rangle = \frac{x_1 + x_2 + \ldots + x_N}{N} = \frac{1}{N} \sum_{i=1}^N x_i$$

The n^{*th*} *moment*:

$$\langle x^n \rangle = \frac{x_1^n + x_2^n + \ldots + x_N^n}{N} = \frac{1}{N} \sum_{i=1}^N x_i^i$$

Standard deviation:

$$\sigma_{x} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left(x_{i} - \langle x \rangle \right)^{2}}$$

Distribution of x:

$$p_x = \frac{1}{N} \sum_i \delta_{x, x_i}$$

where p_x follows

$$\sum_{i} p_x = 1 \left(\int p_x \, dx = 1 \right)$$

AVERAGE DEGREE



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DEGREE DISTRIBUTION

Degree distribution

P(k): probability that a randomly chosen node has degree *k*



a.

C.



 $P(k) = N_k / N$ **9** plot





DEGREE DISTRIBUTION



Discrete Representation: $\mathbf{p}_{\mathbf{k}}$ is the probability that a node has degree \mathbf{k} .

Continuum Description: **p(k)** is the pdf of the degrees, where

$$\int_{k_1}^k p(k) dk$$

represents the probability that a node's degree is between \mathbf{k}_1 and \mathbf{k}_2 .

Normalization condition:

$$\sum_{0}^{\infty} p_{k} = 1 \qquad \qquad \int_{K_{\min}}^{\infty} p(k) dk = 1$$

where K_{min} is the minimal degree in the network.

Adjacency matrix

ADJACENCY MATRIX

A_{ii}=1 if there is a link between node *i* and *j* **A**_{ii}**=0** if nodes *i* and *j* are not connected to each other. $A_{ij} = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \quad A_{ij} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}$

Note that for a directed graph (right) the matrix is not symmetric.

- $A_{ij} = 1$ if there is a link pointing from node *j* and *i*
- $A_{ij} = 0$ if there is no link pointing from *j* to *i*.

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ADJACENCY MATRIX AND NODE DEGREES









 $L = \frac{1}{2} \sum_{i=1}^{N} k_i = \frac{1}{2} \sum_{i=1}^{N} A_{ij}$

Directed



$$A_{ij} = \left(\begin{array}{rrrrr} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{array}\right)$$

$$\begin{array}{c} A_{ij} \neq A_{ji} \\ A_{ii} = 0 \end{array}$$

$$k_i^{in} = \sum_{j=1}^N A_{ij}$$



 $L = \sum_{i=1}^{N} k_{i}^{in} = \sum_{j=1}^{N} k_{j}^{out} = \sum_{i,j}^{N} A_{ij}$

ADJACENCY MATRIX



Real networks are sparse

The maximum number of links a network of N nodes can have is: $L_{\text{max}} = {N \choose 2} = \frac{N(N-1)}{2}$



Most networks observed in real systems are sparse:

L << L_{max} or <k> <<N-1.

WWW (ND Sample):	N=325,729;	L=1.4 10 ⁶	$L_{max} = 10^{12}$	<k>=4.51</k>
Protein (S. Cerevisiae):	N= 1,870;	L=4,470	$L_{max} = 10^7$	<k>=2.39</k>
Coauthorship (Math):	N= 70,975;	L=2 10 ⁵	$L_{max} = 3 \ 10^{10}$	<k>=3.9</k>
Movie Actors:	N=212,250;	L=6 10 ⁶	L _{max} =1.8 10 ¹³	<k>=28.78</k>

(Source: Albert, Barabasi, RMP2002)

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WEIGHTED AND UNWEIGHTED NETWORKS

WEIGHTED AND UNWEIGHTED NETWORKS

$$A_{ij} = w_{ij}$$

GRAPHOLOGY 1



protein-protein interactions, www



Call Graph, metabolic networks

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GRAPHOLOGY 3

Complete Graph

(undirected)



$$A_{ij} = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$



$$A_{ii} = 0 \qquad A_{i \neq j} = 1$$
$$L = L_{\max} = \frac{N(N-1)}{2} \qquad < k >= N-1$$

Actor network, protein-protein interactions

METCALFE'S LAW



BIPARTITE NETWORKS

BIPARTITE GRAPHS

bipartite graph (or **bigraph**) is a <u>graph</u> whose nodes can be divided into two <u>disjoint sets</u> *U* and *V* such that every link connects a node in *U* to one in *V*; that is, *U* and *V* are <u>independent sets</u>.



GENE NETWORK – DISEASE NETWORK



Gene network





Disease network

Goh, Cusick, Valle, Childs, Vidal & Barabási, PNAS (2007)

Ingredient-Flavor Bipartite Network



Y.-Y. Ahn, S. E. Ahnert, J. P. Bagrow, A.-L. Barabási EF lavor network and the principles of food pairing, Scientific Reports 196, (2011).

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PATHOLOGY

PATHS

A path is a sequence of nodes in which each node is adjacent to the next one

 $P_{i0,in}$ of length *n* between nodes i_0 and i_n is an ordered collection of *n*+1 nodes and *n* links

$$P_n = \{i_0, i_1, i_2, \dots, i_n\} \qquad P_n = \{(i_0, i_1), (i_1, i_2), (i_2, i_3), \dots, (i_{n-1}, i_n)\}$$



• In a directed network, the path can follow only the direction of an arrow.



The *distance (shortest path, geodesic path)* between two nodes is defined as the number of edges along the shortest path connecting them.

*If the two nodes are disconnected, the distance is infinity.



In directed graphs each path needs to follow the direction of the arrows.

Thus in a digraph the distance from node A to B (on an AB path) is generally different from the distance from node B to A (on a BCA path).

CONNECTEDNESS

CONNECTIVITY OF UNDIRECTED GRAPHS

Connected (undirected) graph: any two vertices can be joined by a path. A disconnected graph is made up by two or more connected components.



Bridge: if we erase it, the graph becomes disconnected.

The adjacency matrix of a network with several components can be written in a blockdiagonal form, so that nonzero elements are confined to squares, with all other elements being zero:



CONNECTIVITY OF DIRECTED GRAPHS

Strongly connected directed graph: has a path from each node to every other node and vice versa (e.g. AB path and BA path). Weakly connected directed graph: it is connected if we disregard the edge directions.

Strongly connected components can be identified, but not every node is part of a nontrivial strongly connected component.



In-component: nodes that can reach the scc, Out-component: nodes that can be reached from the scc.

Finding the Connected Components of a Network

- 1. Start from a randomly chosen node *i* and perform a BFS (BOX 2.5). Label all nodes reached this way with n = 1.
- 2. If the total number of labeled nodes equals *N*, then the network is connected. If the number of labeled nodes is smaller than *N*, the network consists of several components. To identify them, proceed to step 3.
- Increase the label n → n + 1. Choose an unmarked node j, label it with n. Use BFS to find all nodes reachable from j, label them all with n. Return to step 2.
Clustering coefficient

***** Clustering coefficient:

what fraction of your neighbors are connected?

- * Node i with degree ki
- * C_i in [0,1]









***** Clustering coefficient:

what fraction of your neighbors are connected?

- * Node i with degree ki
- * C_i in [0,1]









Clustering coefficient and Global clustering coefficient

what fraction of your neighbors are connected?

- * Node i with degree k_i
- * C_i in [0,1]





Clustering coefficient and Global clustering coefficient

what fraction of your neighbors are connected?

- * Node i with degree k_i
- * C_i in [0,1]







summary

THREE CENTRAL QUANTITIES IN NETWORK SCIENCE

Degree distribution: P(k)

Path length:

<d>

Clustering coefficient:





Actor network, protein-protein interactions



WWW, citation networks



protein-protein interactions, www



Call Graph, metabolic networks



Protein interaction network, www



Social networks, collaboration networks

Complete Graph

(undirected)



$$A_{ij} = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$



$$L = L_{\max} = \frac{N(N-1)}{2} \quad < k >= N-1$$

Actor network, protein-protein interactions

 $A_{...} = 0$



WWW > directed multigraph with self-interactions

Protein Interactions > undirected unweighted with self-interactions

Collaboration network >

undirected multigraph or weighted.

Mobile phone calls >

directed, weighted.

Facebook Friendship links >

undirected, unweighted.

THREE CENTRAL QUANTITIES IN NETWORK SCIENCE



- A. Degree distribution:
- **B.** Path length:
- **C. Clustering coefficient:**

 $p_{k} = \{0.25; 0.5; 0.25\}$ <d>= 1.33 $C_{i} = \frac{2e_{i}}{k_{i}(k_{i} - 1)}$ Network Science: Graph Theory



GENOME

protein-gene interactions

PROTEOME

protein-protein interactions

METABOLISM

Bio-chemical reactions

Metabolic Network





u



$$d_{max}=14$$

<d>=5.61



	\geq							1 3 All e No	2 4 All edges No cycles		are bridges	
	\geq	\leq		N=8, E=16		N=	8, E=10	7	8 N:	=8,	E=7	
Node	deg	сс	p p	paths	deg	сс	paths		deg	сс	paths	
	1	3	1	3*1+2*2+2*3=13	3	0.33	3*1+2*2+2	*3=13	2	0	2*1+2*2+3+4+5=18	
	2	3	1	3*1+2*2+2*3=13	2	1	2*1+2*2+2*3	+4=16	2	0	2*1+2+3+4+5+6=22	
	3	5	0.6	5*1+2*2=9	2	0	2*1+4*2	+3=13	2	0	2*1+2*2+2*3+4=16	
	4	5	0.6	5*1+2*2=9	3	0.33	3*1+2*2+2	*3=13	1	0	1+2+3+4+5+6+7=28	
	5	5	0.6	5*1+2*2=9	2	0	2*1+4*2	+3=13	2	0	2*1+2*2+2*3+4=16	
	6	5	0.6	5*1+2*2=9	3	0.33	3*1+2*2+2	*3=13	2	0	2*1+2*2+3+4+5=18	
	7	3	1	3*1+2*2+2*3=13	3	0.33	3*1+2*2+2	*3=13	1	0	1+2+3+4+5+6+7=28	
	8	3	1	3*1+2*2+2*3=13	2	1	2*1+2*2+2*3	+4=16	2	0	2*1+2+3+4+5+6=22	
ave		4	0.8	1.571428571	2.5	0.33	1.9285	71429	1.75	0	3	
max		5	1	3	3	1		4	2	0	7	

Introduction

RANDOM NETWORK MODEL



The random network model

RANDOM NETWORK MODEL

Pál Erdös (1913-1996)



Erdös-Rényi model (1960)

Connect with probability p

p=<mark>1/6</mark> N=10 <k> ~ 1.5 Alfréd Rényi (1921-1970)



Network Science: Random Networks

Definition:

A **random graph** is a graph of N nodes where each pair of nodes is connected by probability **p**.

G(N, L) Model

N labeled nodes are connected with *L* randomly placed links. Erdős and Rényi used this definition in their string of papers on random networks [2-9].

G(N, p) Model

Each pair of N labeled nodes is connected with probability *p*, a model introduced by Gilbert [10].

RANDOM NETWORK MODEL

p=1/6 N=12



p=0.03 N=100



The number of links is variable

RANDOM NETWORK MODEL

p=1/6 N=12



p=0.03 N=100



The number of links is variable

RANDOM NETWORK MODEL

p=1/6 N=12



P(L): the probability to have exactly L links in a network of N nodes and probability p:



Binomial distribution...

MATH TUTORIAL Binomial Distribution: The bottom line

$$P(x) = \binom{N}{x} p^{x} (1-p)^{N-x}$$

< x >= Np

$$< x^{2} >= p(1-p)N + p^{2}N^{2}$$

$$\sigma_x = (\langle k^2 \rangle - \langle k \rangle^2)^{1/2} = [p(1-p)N]^{1/2}$$

http://keral2008.blogspot.com/2008/10/derivation-of-mean-and-variance-of.html

Network Science: Random Networks

RANDOM NETWORK MODEL

P(L): the probability to have a network of exactly L links

$$P(L) = \begin{pmatrix} N \\ 2 \\ L \end{pmatrix} p^{L} (1-p)^{\frac{N(N-1)}{2}-L}$$

•The average number of links <*L*> in a random graph

$$L \ge \sum_{L=0}^{\frac{N(N-1)}{2}} LP(L) = p \frac{N(N-1)}{2} \qquad < k \ge 2L/N = p(N-1)$$

•The standard deviation

<

$$\sigma^2 = p(1-p)\frac{N(N-1)}{2}$$

Network Science: Random Networks

Degree distribution
DEGREE DISTRIBUTION OF A RANDOM GRAPH



$$< k >= p(N-1)$$

 $\sigma_k^2 = p(1-p)(N-1)$
 $\frac{\sigma_k}{< k >} = \left[\frac{1-p}{p}\frac{1}{(N-1)}\right]^{1/2} \approx \frac{1}{(N-1)^{1/2}}$

As the network size increases, the distribution becomes increasingly narrow—we are increasingly confident that the degree of a node is in the vicinity of <k>.

Network Science: Random Networks

DEGREE DISTRIBUTION OF A RANDOM GRAPH

$$P(k) = \binom{N-1}{k} p^{k} (1-p)^{(N-1)-k} \qquad < k >= p(N-1) \qquad p = \frac{}{(N-1)}$$

For large N and small k, we can use the following approximations:

$$\binom{N-1}{k} = \frac{(N-1)!}{k!(N-1-k)!} = \frac{(N-1)(N-1-1)(N-1-2)\dots(N-1-k+1)(N-1-k)!}{k!(N-1-k)!} = \frac{(N-1)^k}{k!}$$

$$\ln[(1-p)^{(N-1)-k}] = (N-1-k)\ln(1-\frac{}{N-1}) = -(N-1-k)\frac{}{N-1} = -(1-\frac{k}{N-1}) = -$$

$$(1-p)^{(N-1)-k} = e^{-\langle k \rangle} \qquad \ln(1+x) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} x^n = x - \frac{x^2}{2} + \frac{x^3}{3} - \dots \quad \text{for} \quad |x| \le 1$$
$$P(k) = \binom{N-1}{k} p^k (1-p)^{(N-1)-k} = \frac{(N-1)^k}{k!} p^k e^{-\langle k \rangle} = \frac{(N-1)^k}{k!} \left(\frac{\langle k \rangle}{N-1}\right)^k e^{-\langle k \rangle} = e^{-\langle k \rangle} \frac{\langle k \rangle^k}{k!}$$

Network Science: Random Networks

POISSON DEGREE DISTRIBUTION

$$P(k) = \binom{N-1}{k} p^{k} (1-p)^{(N-1)-k} \qquad < k >= p(N-1) \qquad p = \frac{}{(N-1)}$$

For large N and small k, we arrive at the Poisson distribution:

$$P(k) = e^{-\langle k \rangle} \frac{\langle k \rangle^k}{k!}$$

DEGREE DISTRIBUTION OF A RANDOM GRAPH

