Network Science

Class 2: Graph Theory (Ch2)

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with
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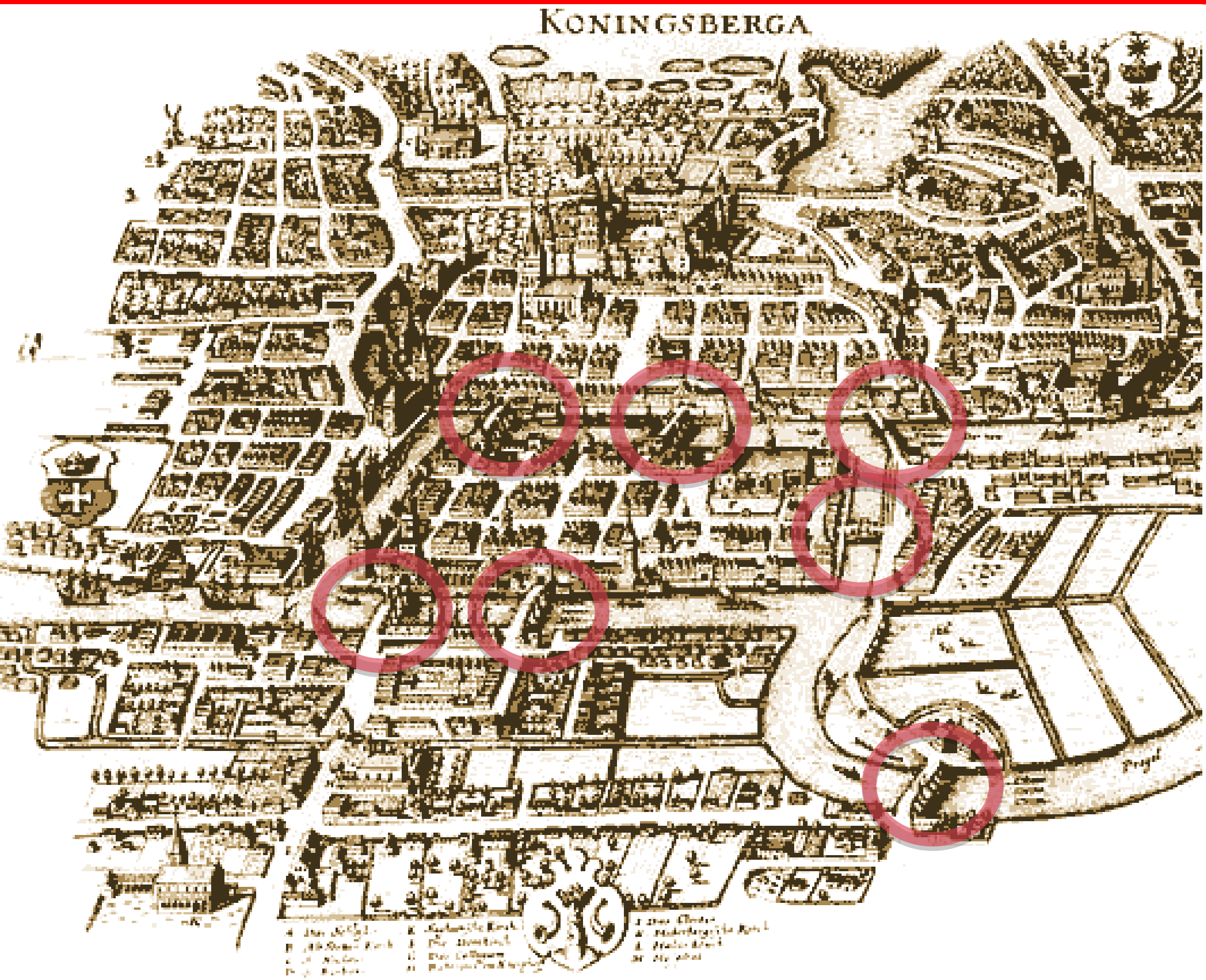
www.BarabasiLab.com

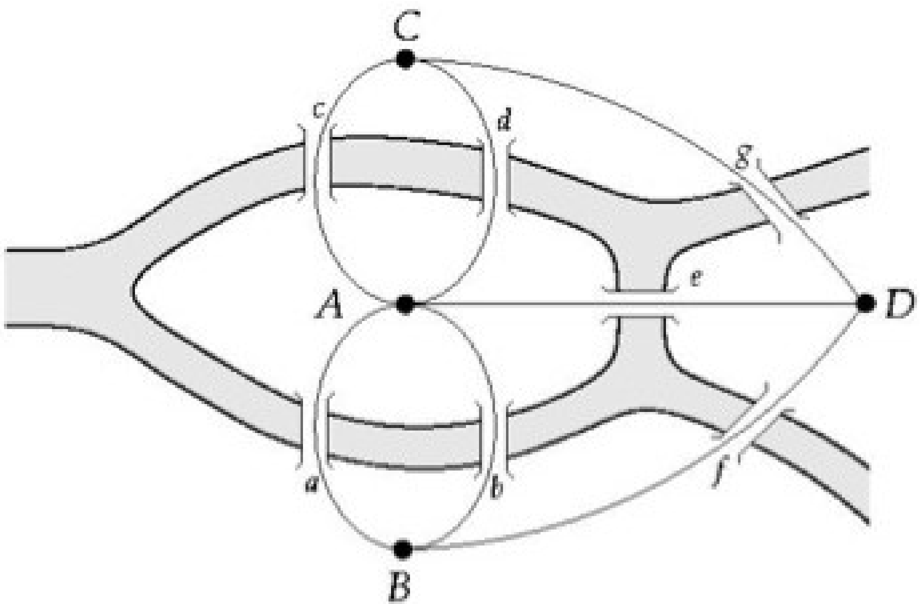
The Bridges of Konigsberg

THE BRIDGES OF KONIGSBERG



Can one walk across the seven bridges and never cross the same bridge twice?

THE BRIDGES OF KONIGSBERG



Can one walk across the seven bridges and never cross the same bridge twice?

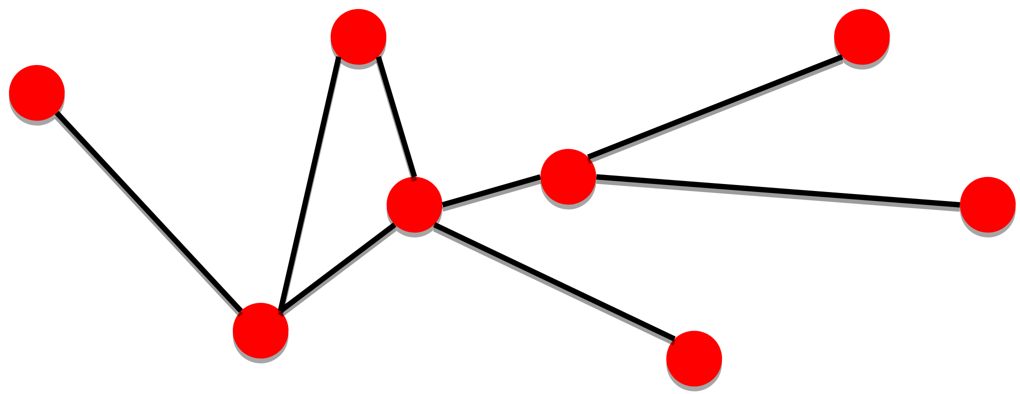
1735: **Euler's theorem:**

a) If a graph has more than two nodes of odd degree, there is no path.

b) If a graph is connected and has no odd degree nodes, it has at least one path.

Networks and graphs

COMPONENTS OF A COMPLEX SYSTEM



- **components**: nodes, vertices N
- **interactions**: links, edges L
- **system**: network, graph (N,L)

NETWORKS OR GRAPHS?

network often refers to real systems

- www,
- social network
- metabolic network.

Language: (Network, node, link)

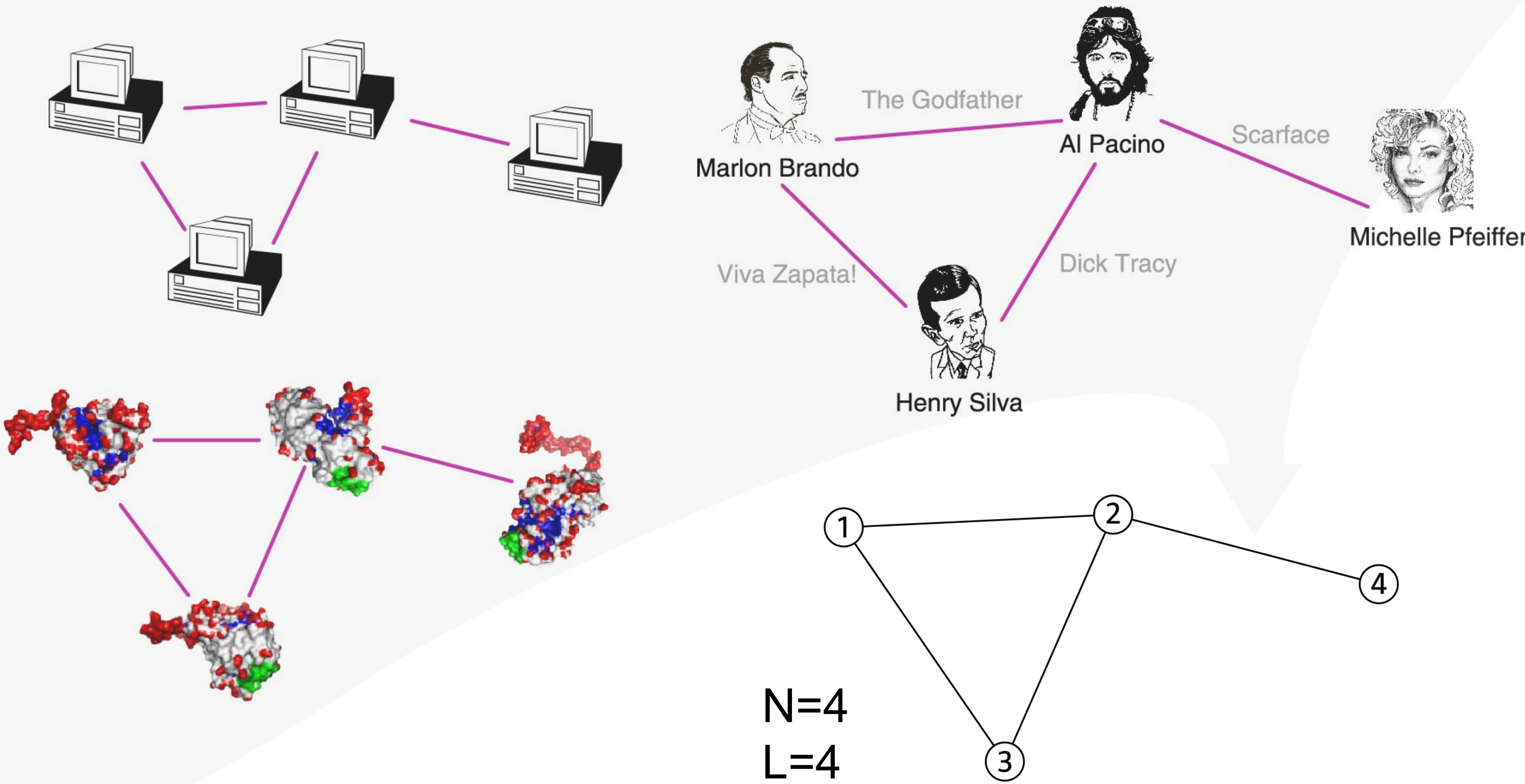
graph: mathematical representation of a network

- web graph,
- social graph (a Facebook term)

Language: (Graph, vertex, edge)

We will try to make this distinction whenever it is appropriate, but in most cases we will use the two terms interchangeably.

A COMMON LANGUAGE



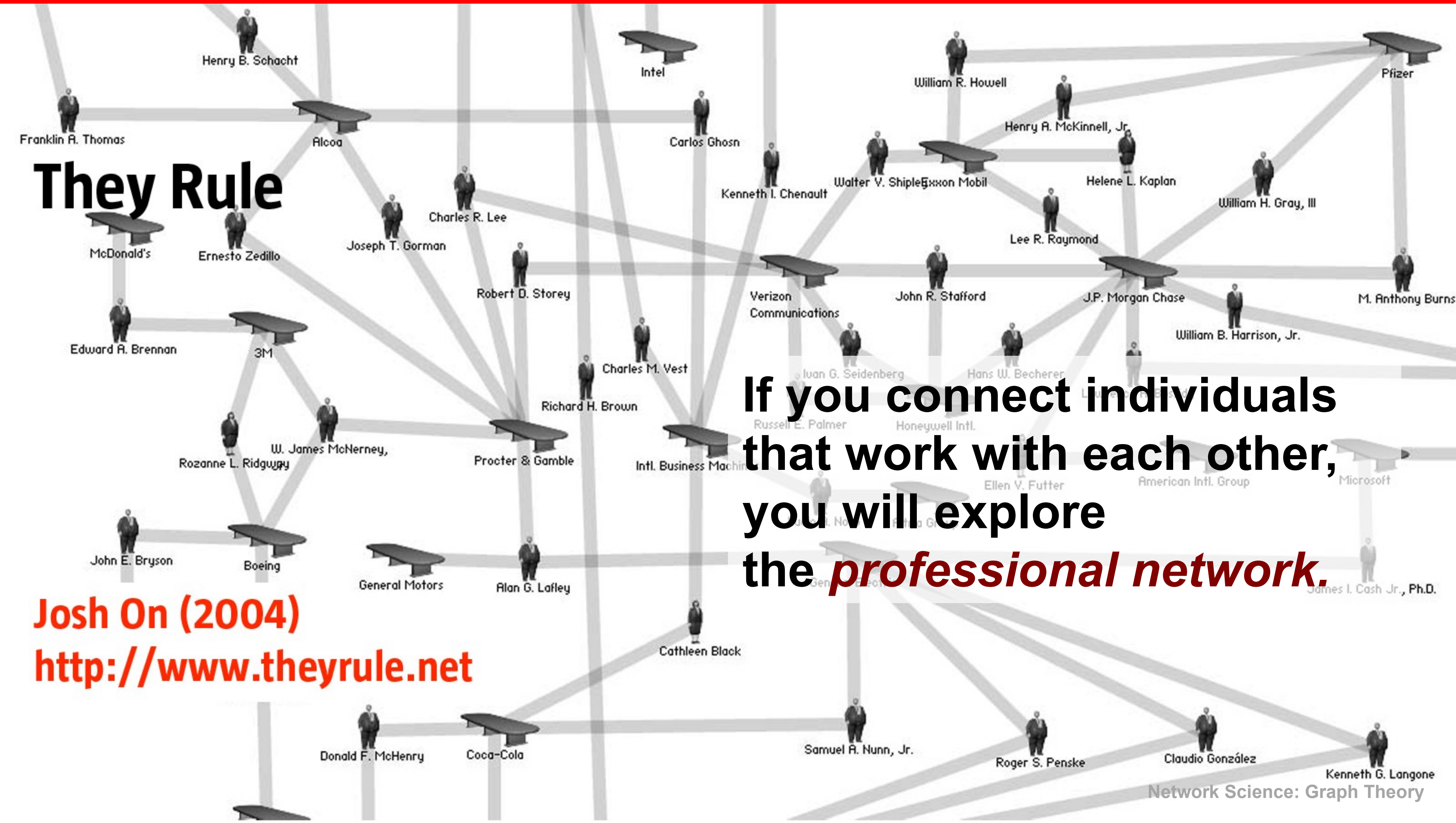
CHOOSING A PROPER REPRESENTATION

The choice of the proper network representation determines our ability to use network theory successfully.

In some cases there is a unique, unambiguous representation. In other cases, the representation is by no means unique.

For example, the way we assign the links between a group of individuals will determine the nature of the question we can study.

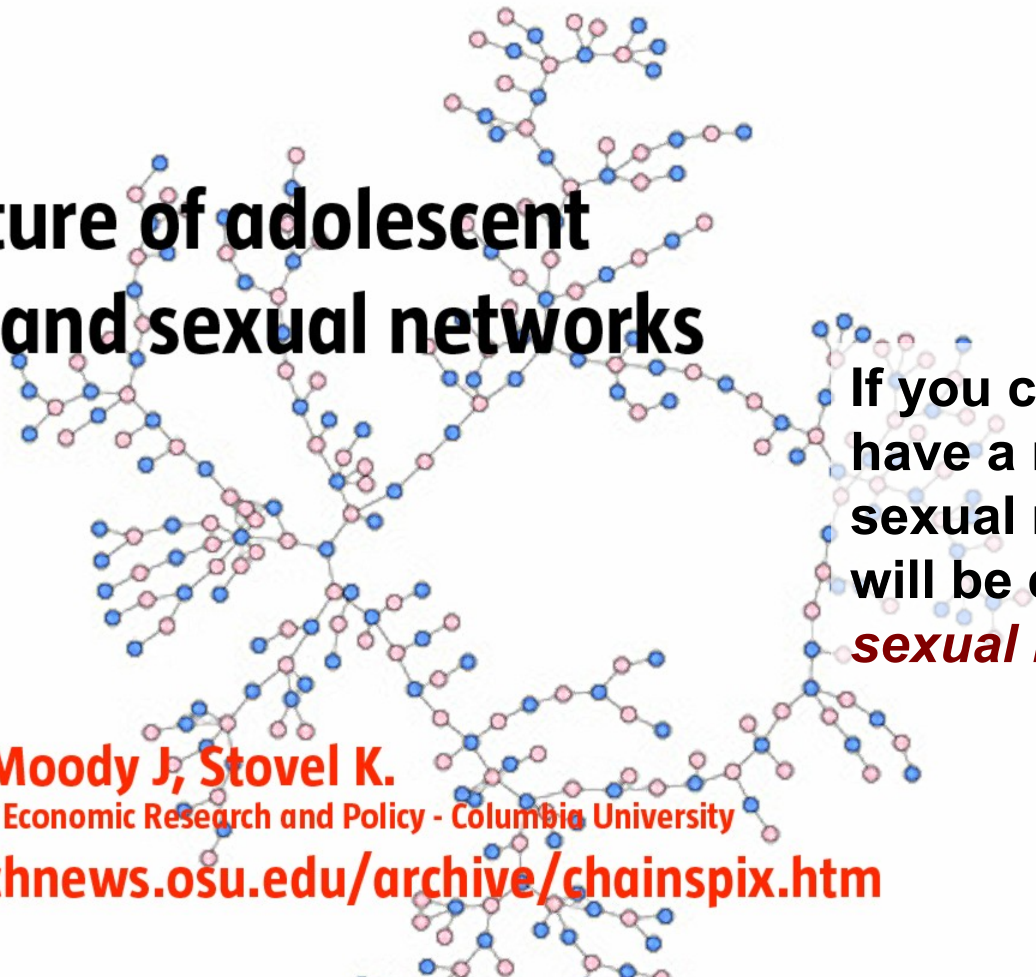
CHOOSING A PROPER REPRESENTATION



They Rule

Josh On (2004)
http://www.theyrule.net

If you connect individuals that work with each other, you will explore the *professional network*.



The structure of adolescent romantic and sexual networks

If you connect those that have a romantic and sexual relationship, you will be exploring the *sexual networks*.

Bearman PS, Moody J, Stovel K.
Institute for Social and Economic Research and Policy - Columbia University

http://researchnews.osu.edu/archive/chainspix.htm

CHOOSING A PROPER REPRESENTATION

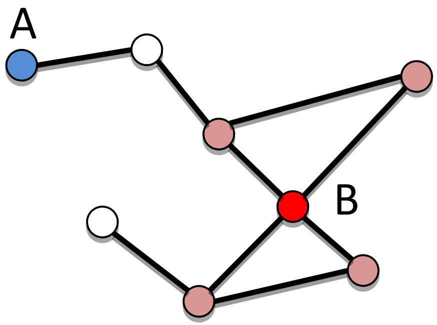
If you connect individuals based on their first name (*all Peters connected to each other*), you will be exploring what?

It is a network, nevertheless.

Degree, Average Degree and Degree Distribution

NODE DEGREES

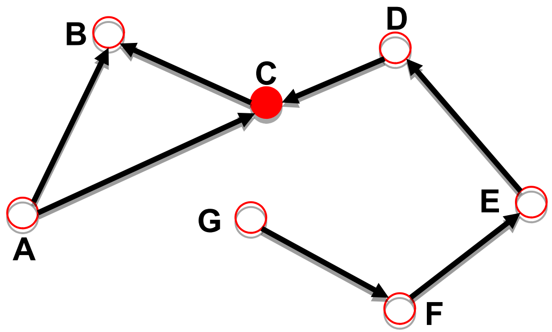
Undirected



Node degree: the number of links connected to the node.

$$k_A = 1 \qquad k_B = 4$$

Directed



In *directed networks* we can define an in-degree and out-degree.

The (total) degree is the sum of in- and out-degree.

$$k_C^{in} = 2 \qquad k_C^{out} = 1 \qquad k_C = 3$$

Source: a node with $k^{in} = 0$; Sink: a node with $k^{out} = 0$.

A BIT OF STATISTICS

BRIEF STATISTICS REVIEW

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

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:

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

Standard deviation:

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

Distribution of x:

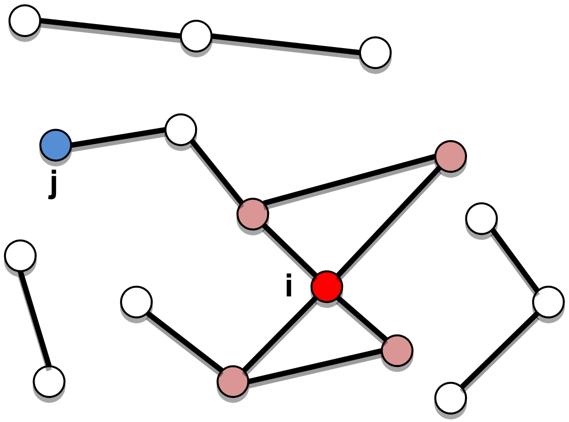
$$p_x = \frac{1}{N}\sum_i \delta_{x,x_i}$$

where p_x follows

$$\sum_i p_x = 1 \left(\int p_x \, dx = 1 \right)$$

AVERAGE DEGREE

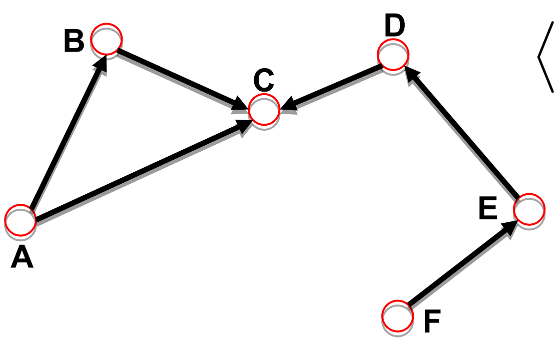
Undirected



$$\langle k \rangle \equiv \frac{1}{N}\sum_{i=1}^{N} k_i \qquad \langle k \rangle \equiv \frac{2L}{N}$$

N – the number of nodes in the graph

Directed



$$\langle k^{in} \rangle \equiv \frac{1}{N}\sum_{i=1}^{N} k_i^{in}, \quad \langle k^{out} \rangle \equiv \frac{1}{N}\sum_{i=1}^{N} k_i^{out}, \quad \langle k^{in} \rangle = \langle k^{out} \rangle$$

$$\langle k \rangle \equiv \frac{L}{N}$$

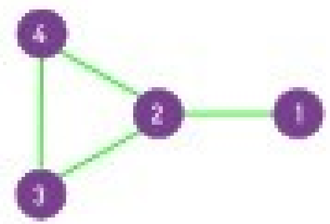
Average Degree

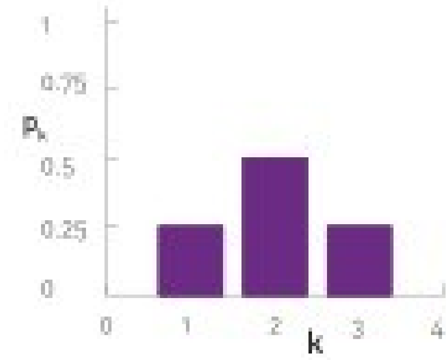
NETWORK	NODES	LINKS	DIRECTED UNDIRECTED	N	L	$\langle k \rangle$
Internet	Routers	Internet connections	Undirected	192,244	609,066	6.33
WWW	Webpages	Links	Directed	325,729	1,497,134	4.60
Power Grid	Power plants, transformers	Cables	Undirected	4,941	6,594	2.67
Mobile Phone Calls	Subscribers	Calls	Directed	36,595	91,826	2.51
Email	Email addresses	Emails	Directed	57,194	103,731	1.81
Science Collaboration	Scientists	Co-authorship	Undirected	23,133	93,439	8.08
Actor Network	Actors	Co-acting	Undirected	702,388	29,397,908	83.71
Citation Network	Paper	Citations	Directed	449,673	4,689,479	10.43
E. Coli Metabolism	Metabolites	Chemical reactions	Directed	1,039	5,802	5.58
Protein Interactions	Proteins	Binding interactions	Undirected	2,018	2,930	2.90

DEGREE DISTRIBUTION

Degree distribution

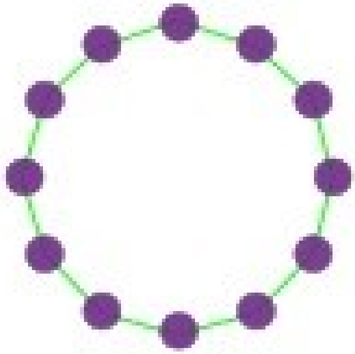
P(k): probability that a randomly chosen node has degree *k*

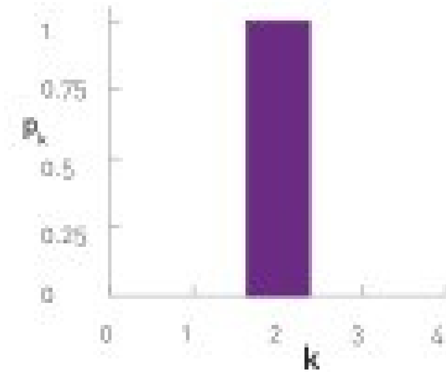




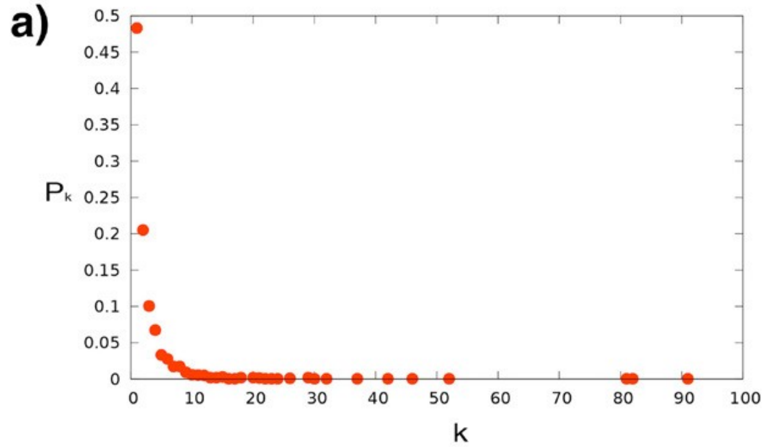
N_k = # nodes with degree k

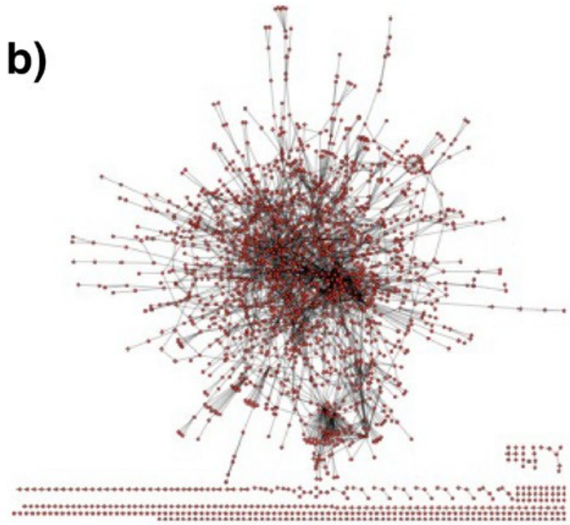
$P(k) = N_k / N$ ➔ plot





DEGREE DISTRIBUTION





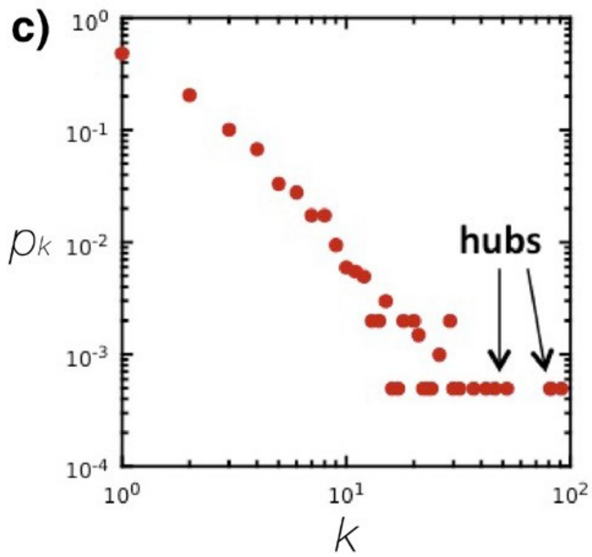


Image 2.4b

DEGREE DISTRIBUTION

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

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

$$\int_{k_1}^{k_2} p(k)dk$$

represents the probability that a node's degree is between $\mathbf{k_1}$ and $\mathbf{k_2}$.

Normalization condition:

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

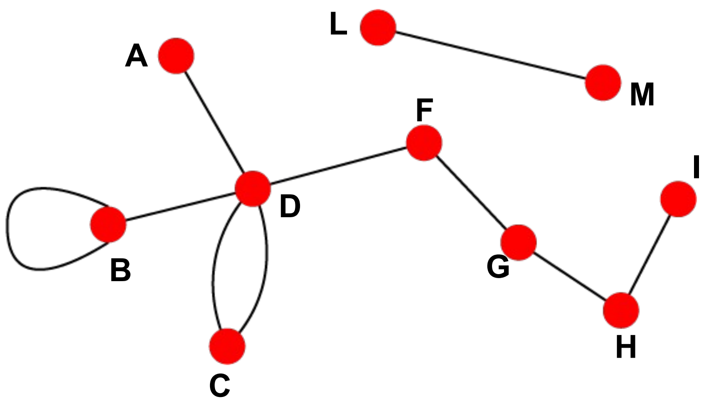
where K_{min} is the minimal degree in the network.

UNDIRECTED VS. DIRECTED NETWORKS

Undirected

Links: undirected (*symmetrical*)

Graph:



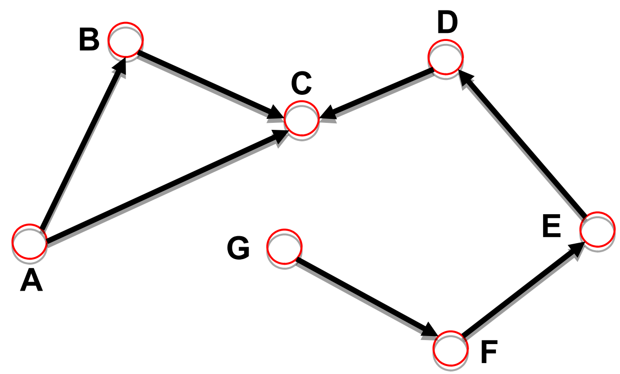
Undirected links :

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

Section 2.2 Reference Networks

NETWORK	NODES	LINKS	DIRECTED UNDIRECTED	N	L
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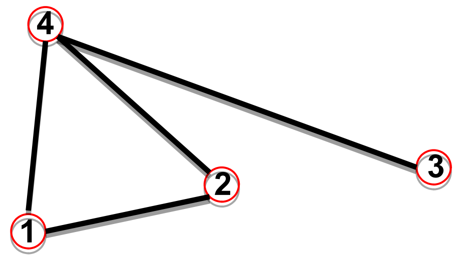
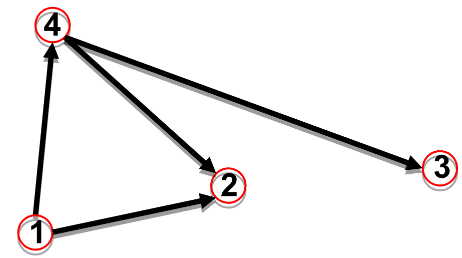
Question 4

Q4: Adjacency Matrices

Adjacency matrix

ADJACENCY MATRIX





A_{ij}**=1** if there is a link between node *i* and *j*

A_{ij}**=0** if nodes *i* and *j* are not connected to each other.

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

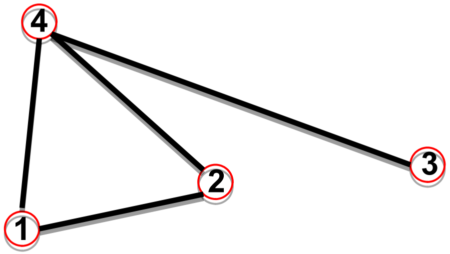
Note that for a directed graph (right) the matrix is not symmetric.

$A_{ij} = 1$ if there is a link pointing from node *j* and *i*

$A_{ij} = 0$ if there is no link pointing from *j* to *i*.

ADJACENCY MATRIX AND NODE DEGREES

Undirected



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

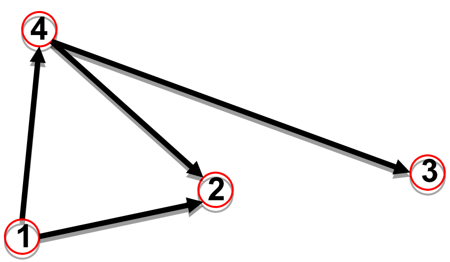
$$A_{ij} = A_{ji}$$
$$A_{ii} = 0$$

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

$$k_j = \sum_{i=1}^{N} A_{ij}$$

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

Directed



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

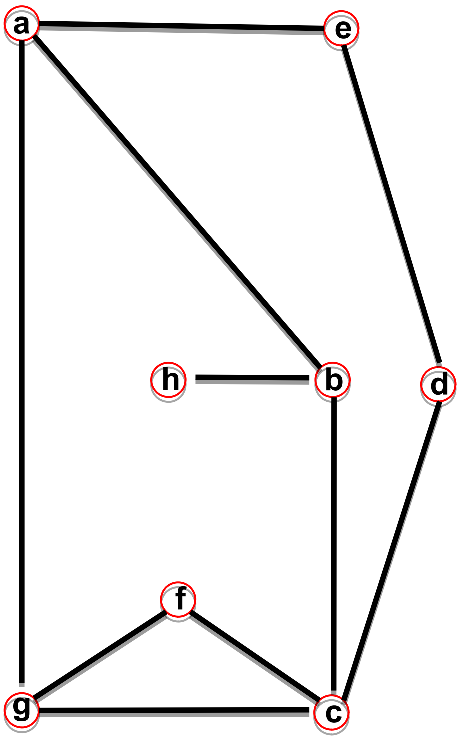
$$A_{ij} \neq A_{ji}$$
$$A_{ii} = 0$$

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

$$k_j^{out} = \sum_{i=1}^{N} A_{ij}$$

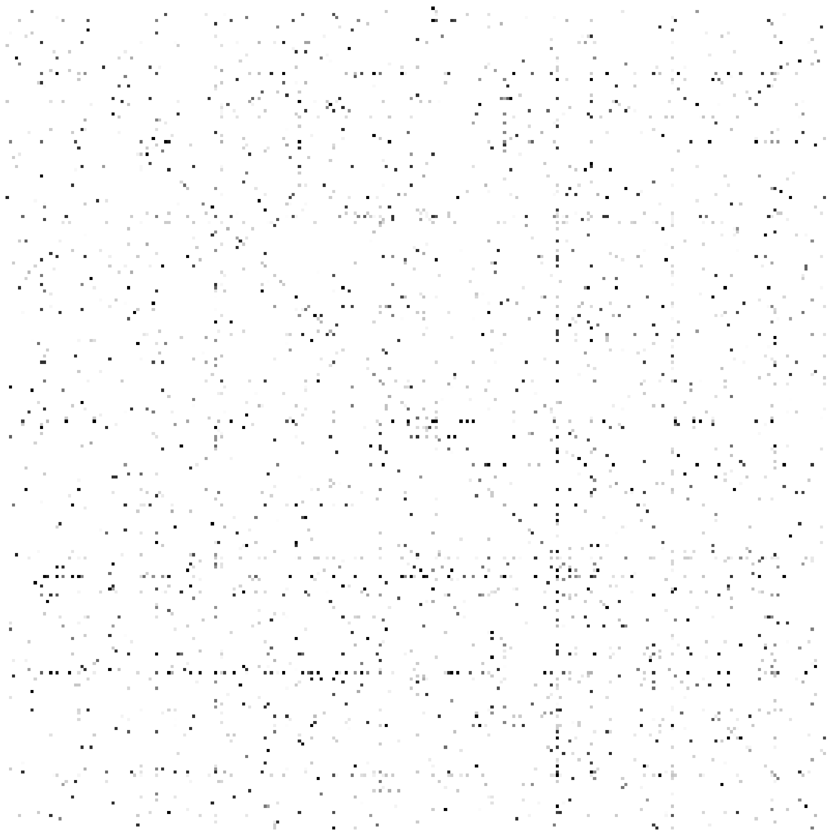
$$L = \sum_{i=1}^{N} k_i^{in} = \sum_{j=1}^{N} k_j^{out} = \sum_{i,j}^{N} A_{ij}$$

ADJACENCY MATRIX



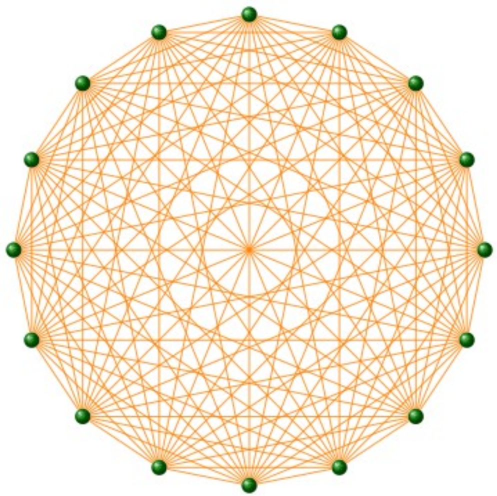
	a	b	c	d	e	f	g	h
a	0	1	0	0	1	0	1	0
b	1	0	1	0	0	0	0	1
c	0	1	0	1	0	1	1	0
d	0	0	1	0	1	0	0	0
e	1	0	0	1	0	0	0	0
f	0	0	1	0	0	0	1	0
g	1	0	1	0	0	0	0	0
h	0	1	0	0	0	0	0	0

ADJACENCY MATRICES ARE SPARSE



Real networks are sparse

COMPLETE GRAPH



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

A graph with degree $L=L_{max}$ is called a complete graph, and its average degree is **<k>=N-1**

REAL NETWORKS ARE SPARSE

Most networks observed in real systems are sparse:

$$L \ll L_{max}$$

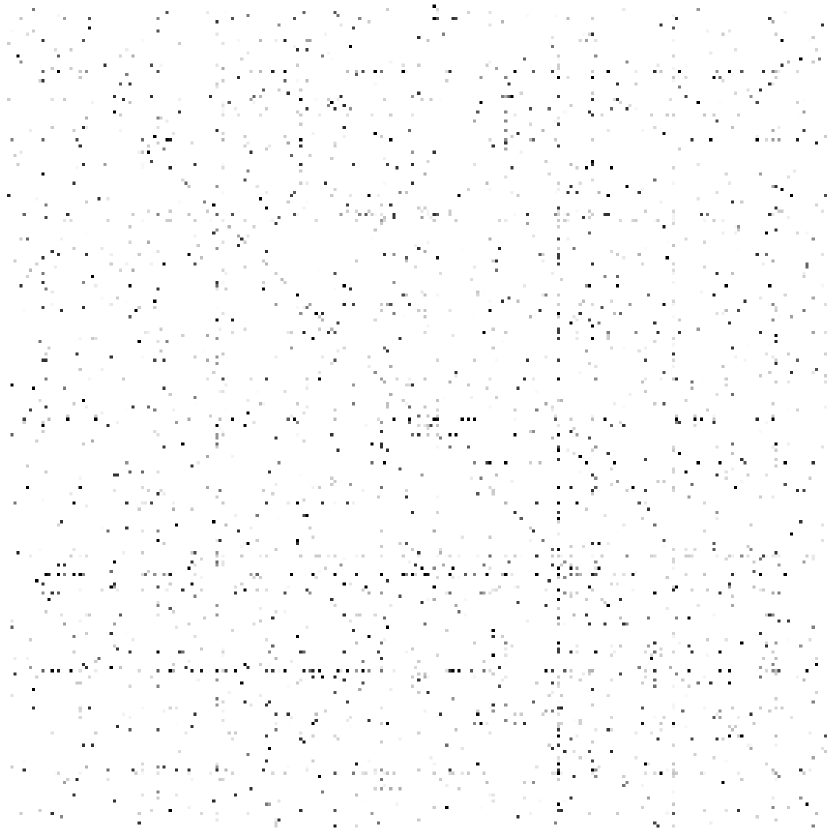
or

$$\langle k \rangle \ll N-1.$$

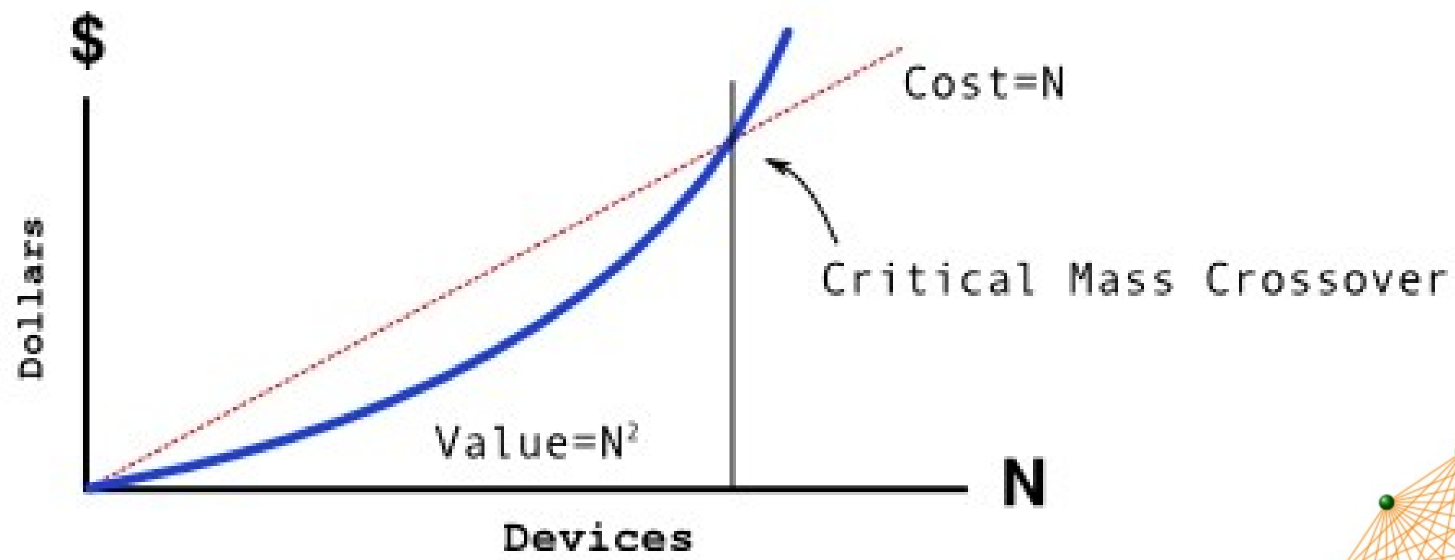
WWW (ND Sample):	N=325,729;	L=1.4 10^6	$L_{max}=10^{12}$	$\langle k \rangle=4.51$
Protein (*S. Cerevisiae*):	N= 1,870;	L=4,470	$L_{max}=10^7$	$\langle k \rangle=2.39$
Coauthorship (Math):	N= 70,975;	L=2 10^5	$L_{max}=3\ 10^{10}$	$\langle k \rangle=3.9$
Movie Actors:	N=212,250;	L=6 10^6	$L_{max}=1.8\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

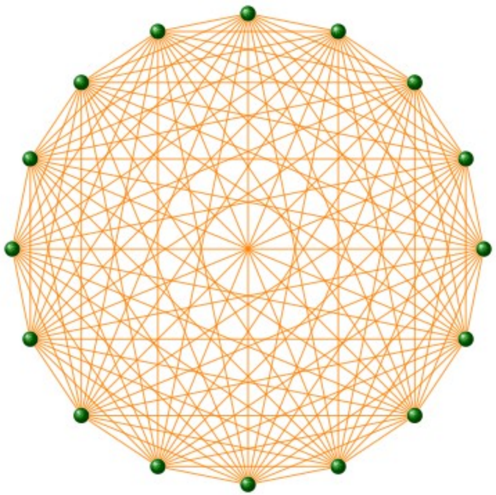
(Source: Albert, Barabasi, RMP2002)

ADJACENCY MATRICES ARE SPARSE



METCALFE'S LAW





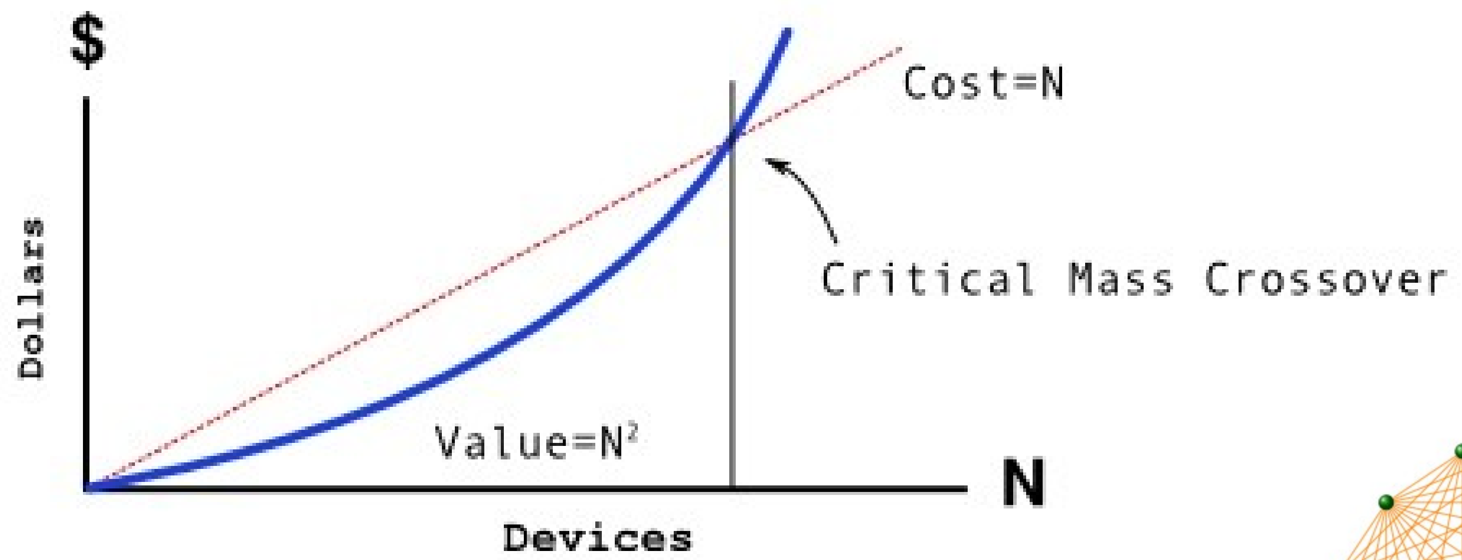
The maximum number of links a network of N nodes can have is: $L_{max} = \binom{N}{2} = \frac{N(N-1)}{2}$

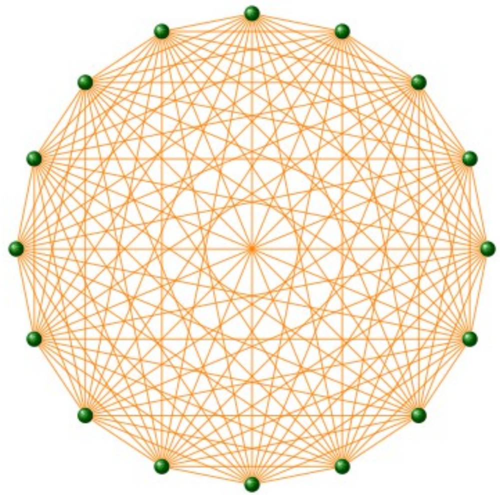
WEIGHTED AND UNWEIGHTED NETWORKS

WEIGHTED AND UNWEIGHTED NETWORKS

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

METCALFE'S LAW



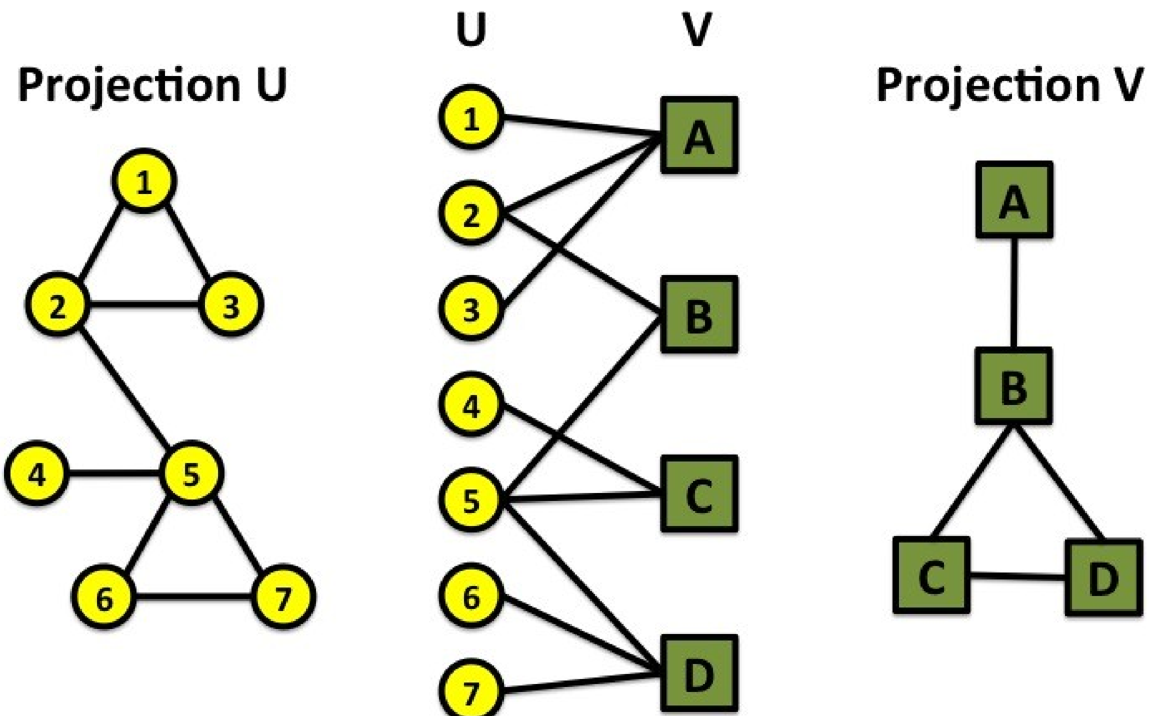


The maximum number of links a network of N nodes can have is: $L_{max} = \binom{N}{2} = \frac{N(N-1)}{2}$

BIPARTITE NETWORKS

BIPARTITE GRAPHS

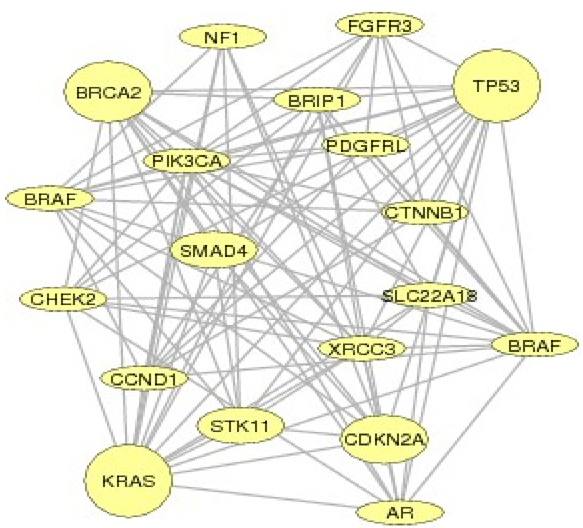
bipartite graph (or **bigraph**) is a graph whose nodes can be divided into two disjoint sets *U* and *V* such that every link connects a node in *U* to one in *V*; that is, *U* and *V* are independent sets.



Examples:

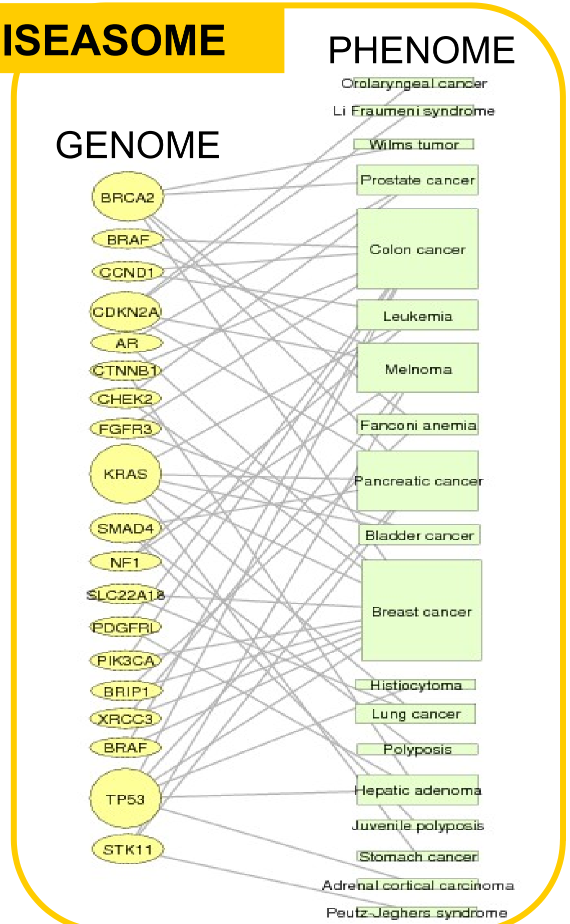
Hollywood actor network
Collaboration networks
Disease network (diseasome)

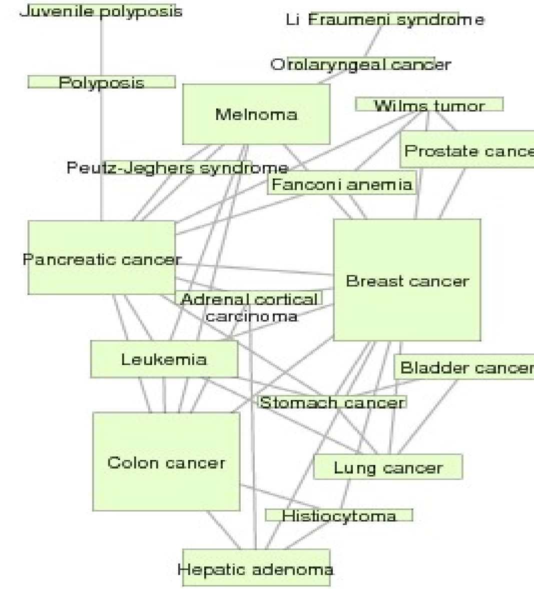
GENE NETWORK – DISEASE NETWORK



Gene network

DISEASOME

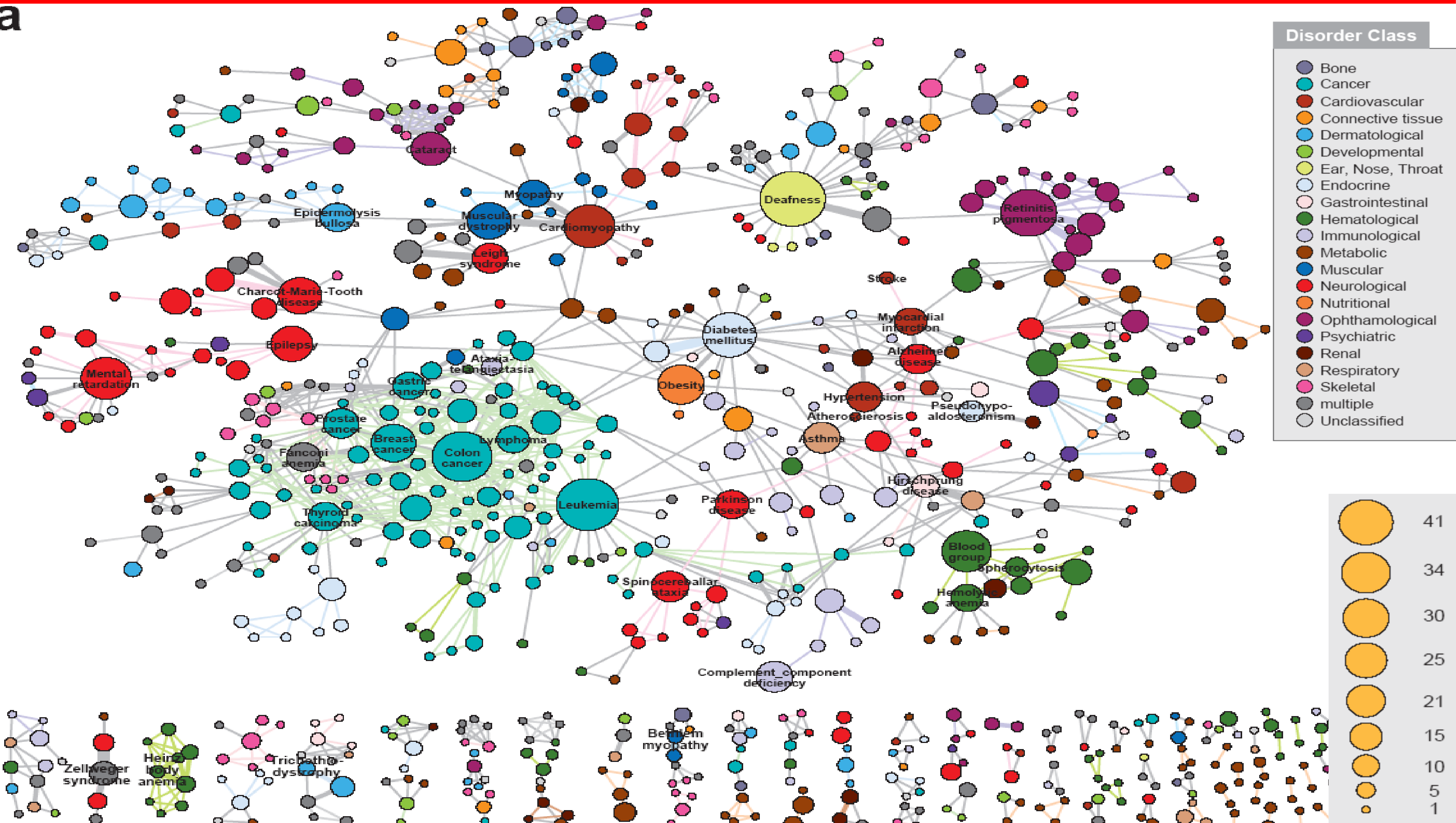




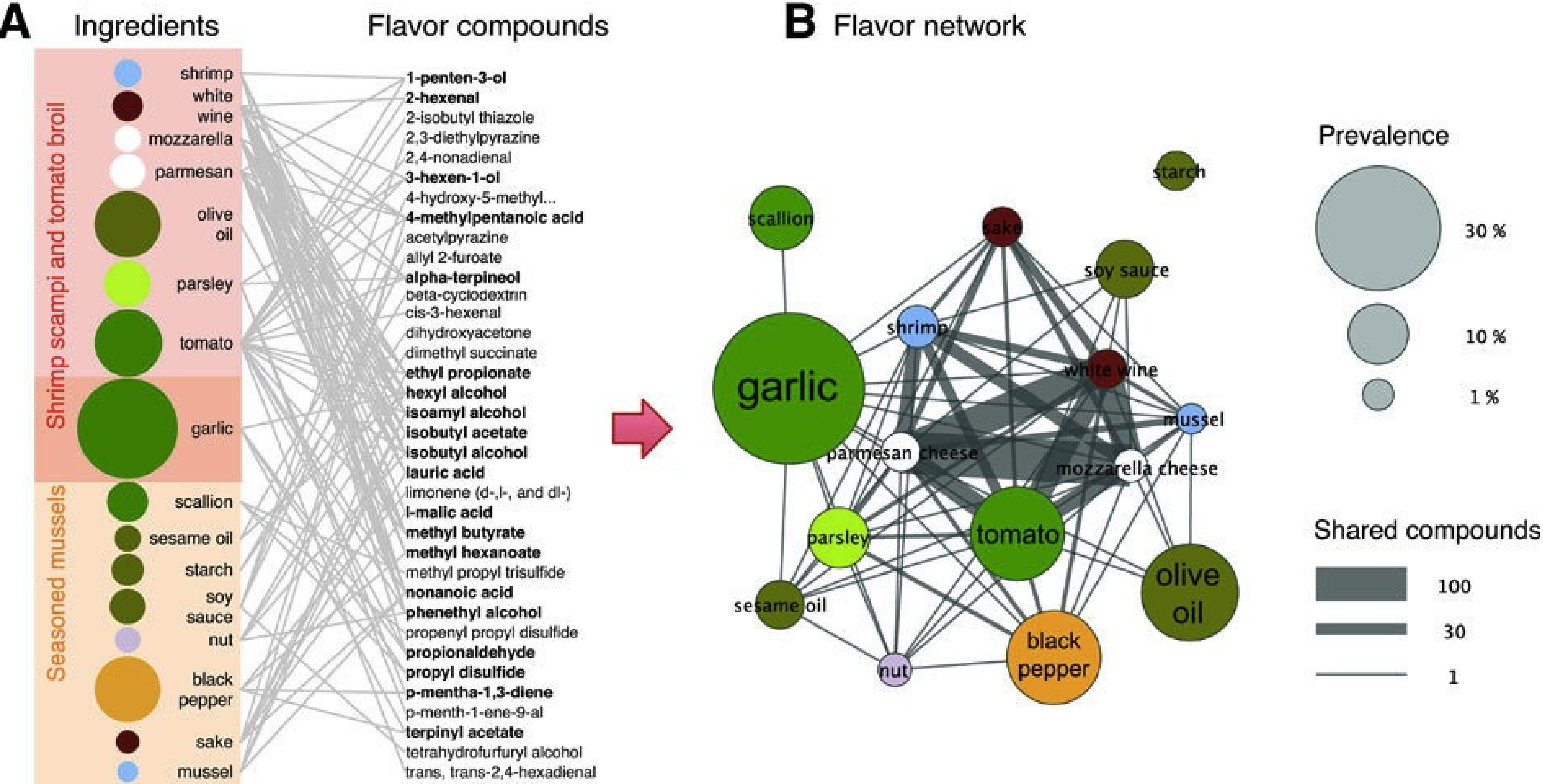
Disease network

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

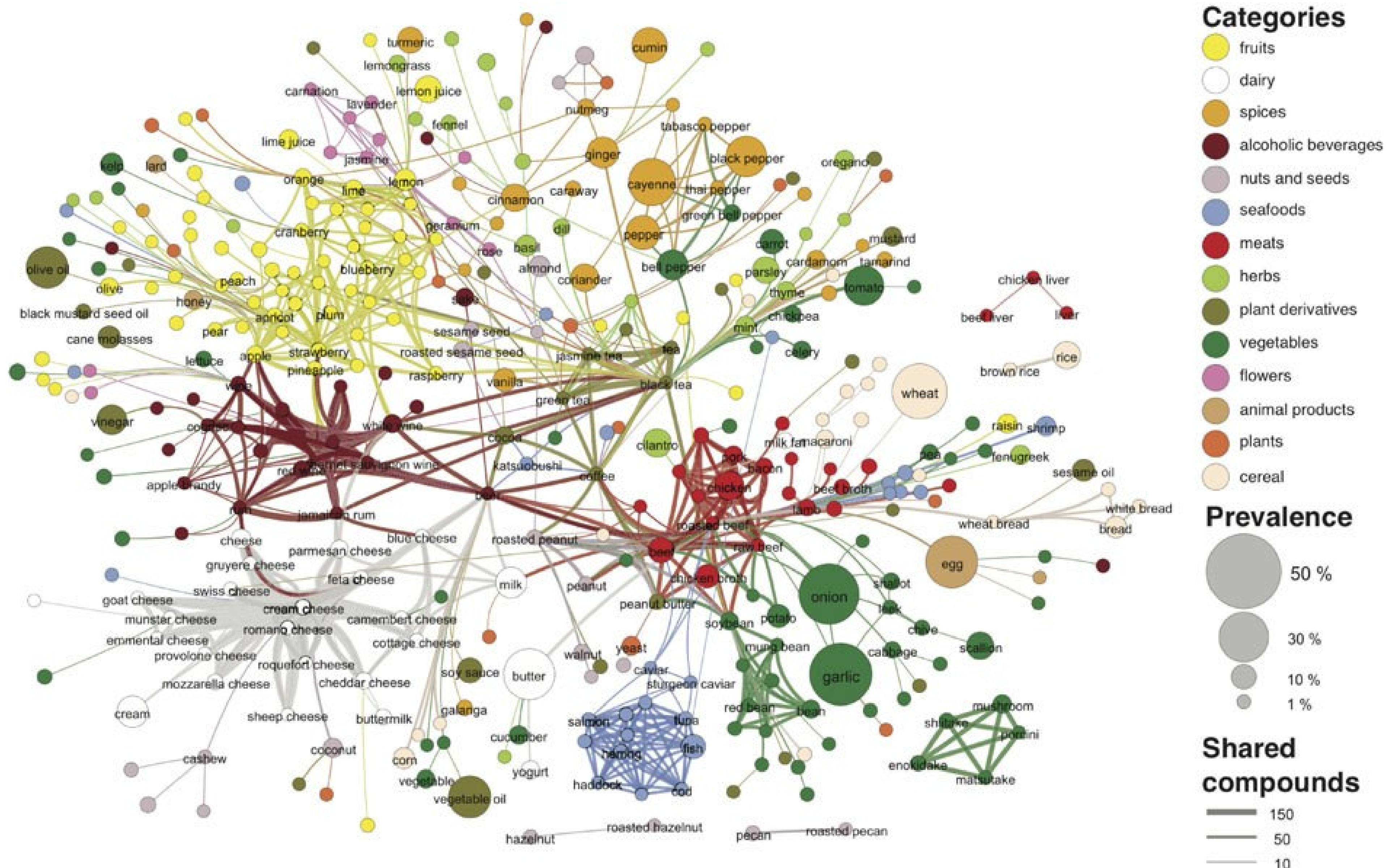
HUMAN DISEASE NETWORK



Ingredient-Flavor Bipartite Network



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



Categories
fruits
dairy
spices
alcoholic beverages
nuts and seeds
seafoods
meats
herbs
plant derivatives
vegetables
flowers
animal products
plants
cereal
Prevalence
50 %
30 %
10 %
1 %
Shared compounds
150
50
10
turmeric
cumin
lemongrass
carnation
lemon juice
lavender
nutmeg
tabasco pepper
fennel
lime juice
jasmine
ginger
black pepper
kelp
lard
orange
lime
lemon
cayenne
caraway
thai pepper
oregano
cinnamon
green bell pepper
geranium
cranberry
dill
pepper
mustard
rose
basil
carrot
olive oil
blueberry
almond
bell pepper
cardamom
tamarind
coriander
parsley
olive
peach
honey
thyme
tomato
sake
chicken liver
black mustard seed oil
apricot
plum
chickpea
beef liver
liver
cane molasses
pear
sesame seed
mint
apple
strawberry
roasted sesame seed
lettuce
jasmine tea
tea
celery
rice
pineapple
raspberry
vanilla
black tea
brown rice
wine
wheat
green tea
vinegar
cognac
white wine
raisin
shrimp
cocoa
cilantro
milk fat
macaroni
pork
fenugreek
pea
bacon
red wine
cabernet sauvignon wine
katsuobushi
sesame oil
coffee
apple brandy
chicken
beef broth
beer
lamb
white bread
rum
jamaican rum
wheat bread
roasted beef
bread
cheese
blue cheese
roasted peanut
beef
raw beef
parmesan cheese
egg
gruyere cheese
feta cheese
chicken broth
milk
peanut
onion
shallot
swiss cheese
goat cheese
cream cheese
peanut butter
leek
munster cheese
camembert cheese
soybean
potato
chive
emmental cheese
romano cheese
cottage cheese
walnut
yeast
mung bean
cabbage
scallion
provolone cheese
roquefort cheese
caviar
soy sauce
butter
garlic
mozzarella cheese
cheddar cheese
sturgeon caviar
mushroom
cream
sheep cheese
buttermilk
galanga
red bean
bean
salmon
tuna
shiitake
porcini
cucumber
cashew
fish
coconut
herring
enokidake
corn
yogurt
matsutake
haddock
cod
vegetable
vegetable oil
roasted hazelnut
hazelnut
pecan
roasted pecan

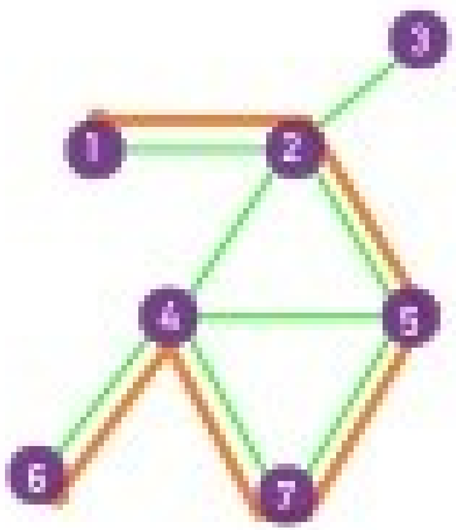
PATHOLOGY

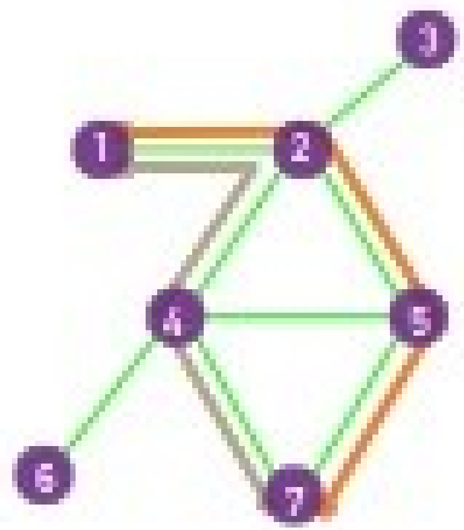
PATHS

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

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

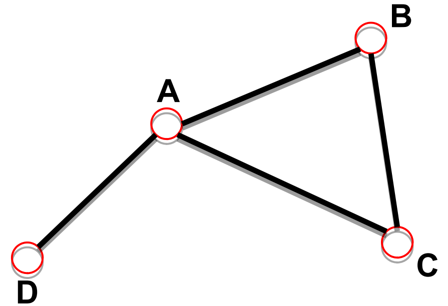




- In a directed network, the path can follow only the direction of an arrow.

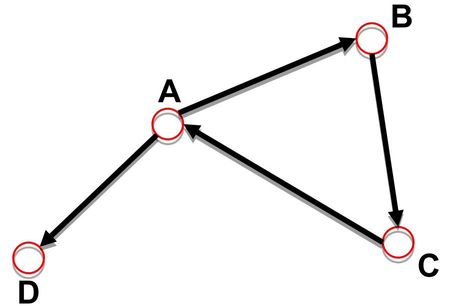
DISTANCE IN A GRAPH

Shortest Path, Geodesic Path



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 BA path).

N_{ij}, number of paths between any two nodes *i* and *j*:

***<u>Length n=1</u>*:** If there is a link between *i* and *j*, then $A_{ij}=1$ and $A_{ij}=0$ otherwise.

<u>Length n=2:</u> If there is a path of length two between *i* and *j*, then $A_{ik}A_{kj}=1$, and $A_{ik}A_{kj}=0$ otherwise.
The number of paths of length 2:

$$N_{ij}^{(2)} = \sum_{k=1}^{N} A_{ik}A_{kj} = [A^2]_{ij}$$

<u>Length n:</u> In general, if there is a path of length *n* between *i* and *j*, then $A_{ik}\ldots A_{lj}=1$ and $A_{ik}\ldots A_{lj}=0$ otherwise.
The number of paths of length *n* between *i* and *j* is*

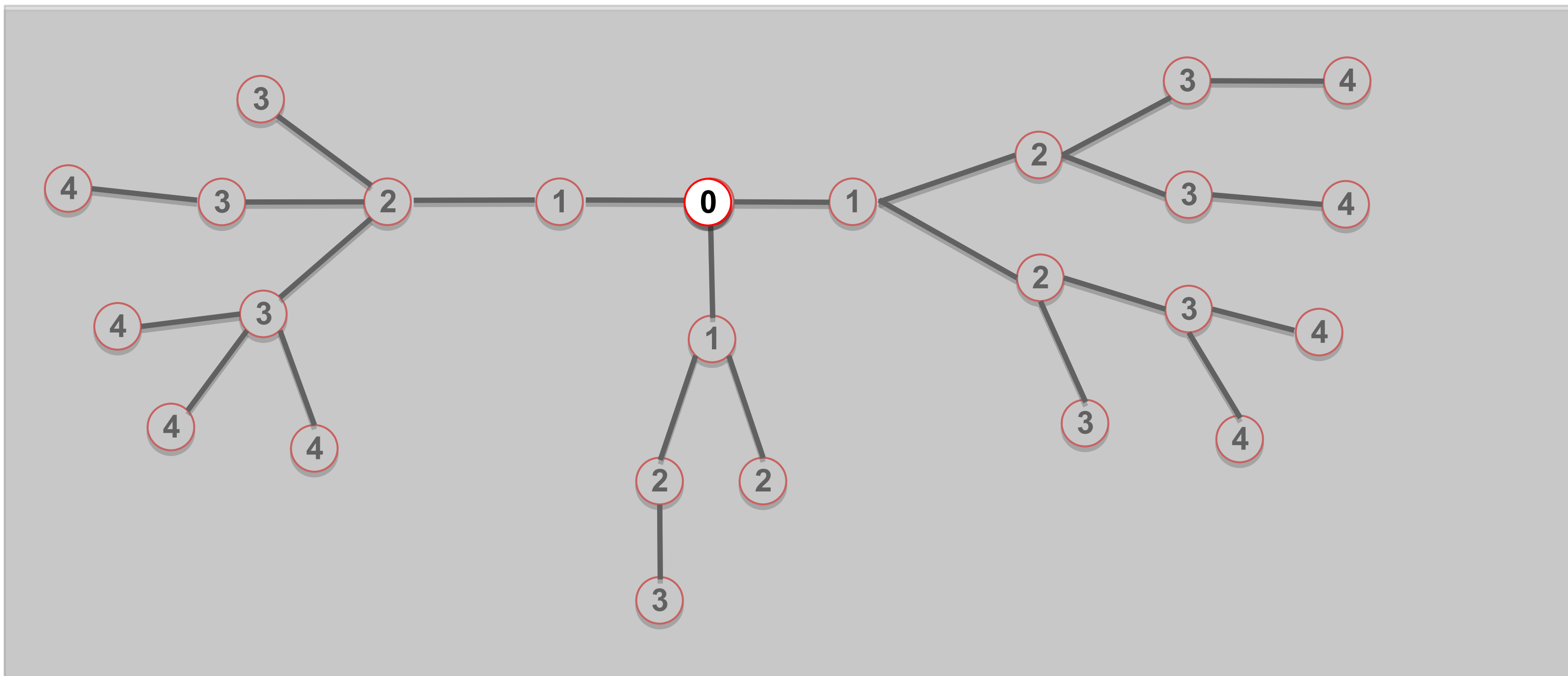
$$N_{ij}^{(n)} = [A^n]_{ij}$$

**holds for both directed and undirected networks.*

FINDING DISTANCES: BREADTH FIRST SEARCH

Distance between node 0 and node 4:

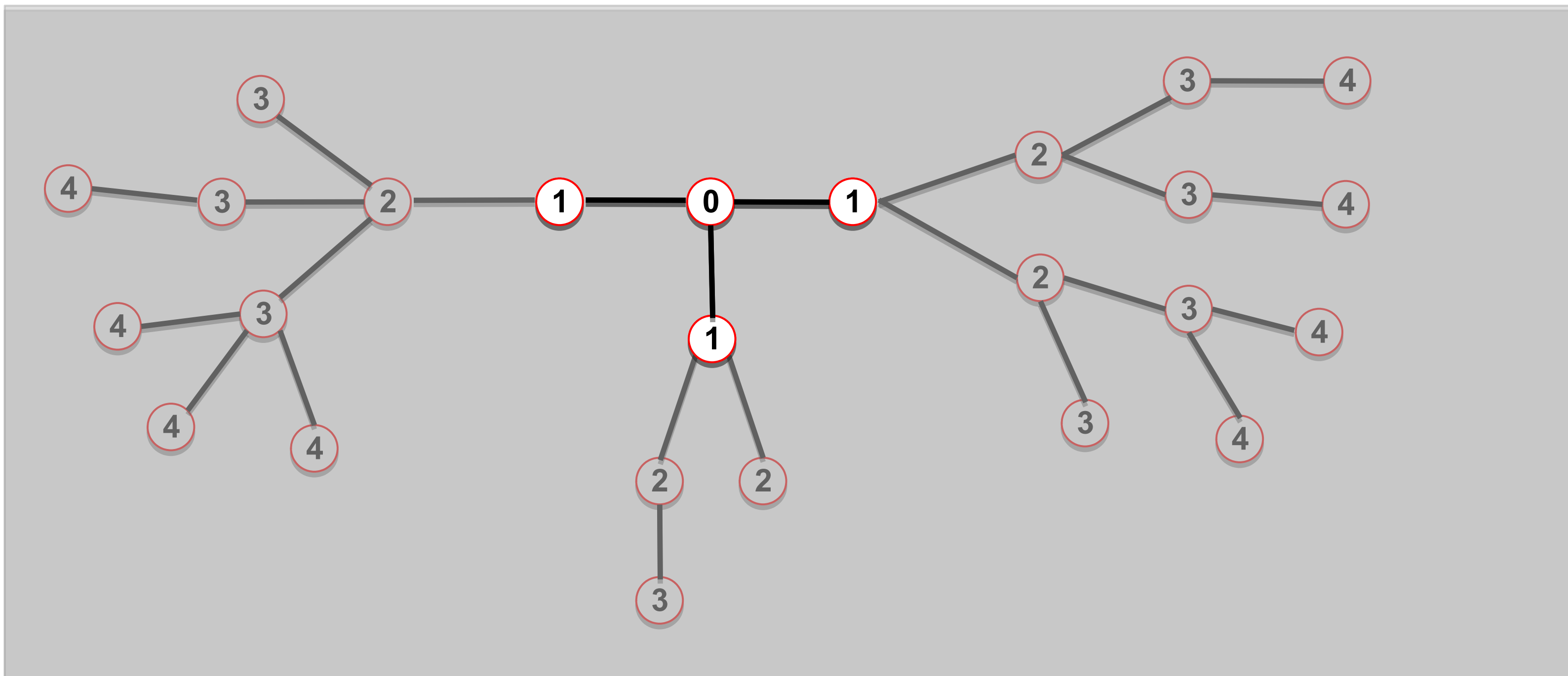
1. Start at 0.



FINDING DISTANCES: BREADTH FIRST SEARCH

Distance between node 0 and node 4:

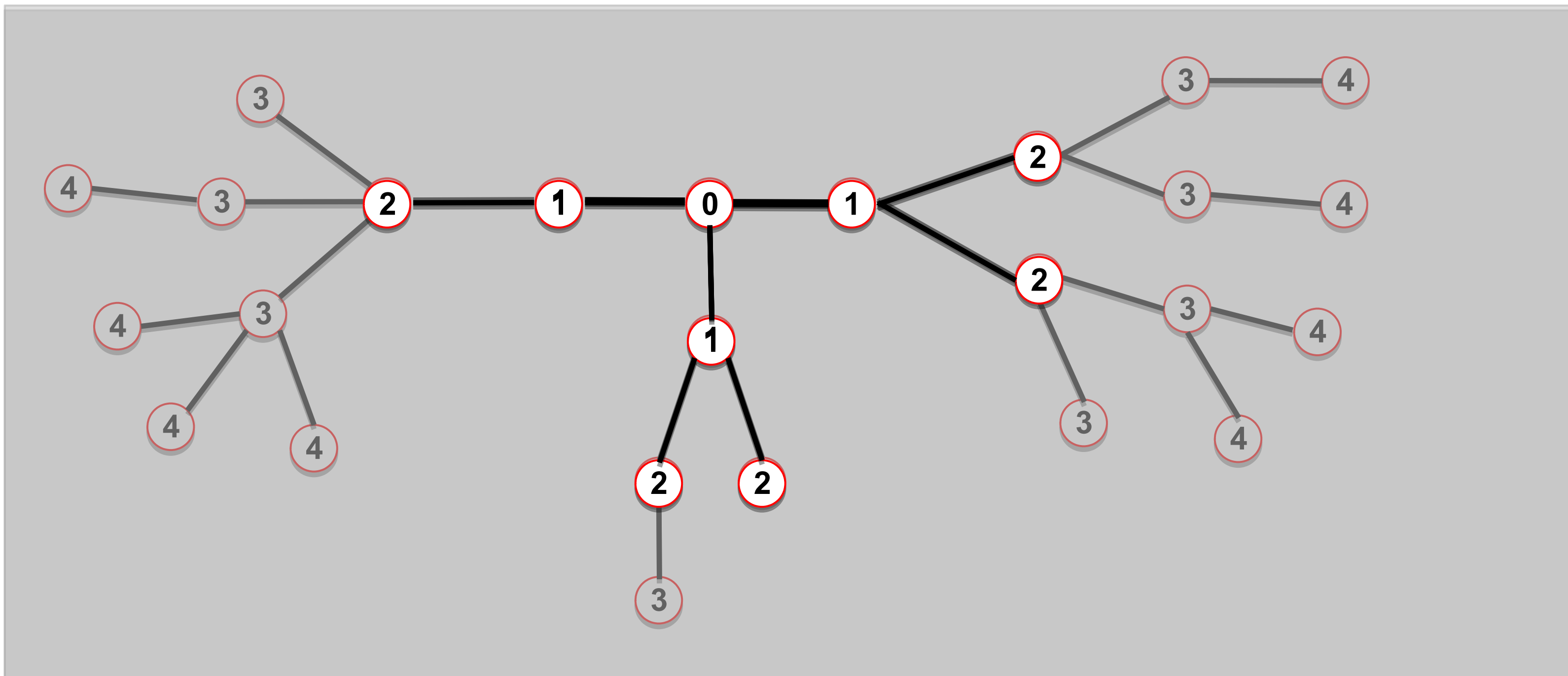
1. Start at 0.
2. Find the nodes adjacent to 1. Mark them as at distance 1. Put them in a queue.



FINDING DISTANCES: BREADTH FIRST SEARCH

Distance between node 0 and node 4:

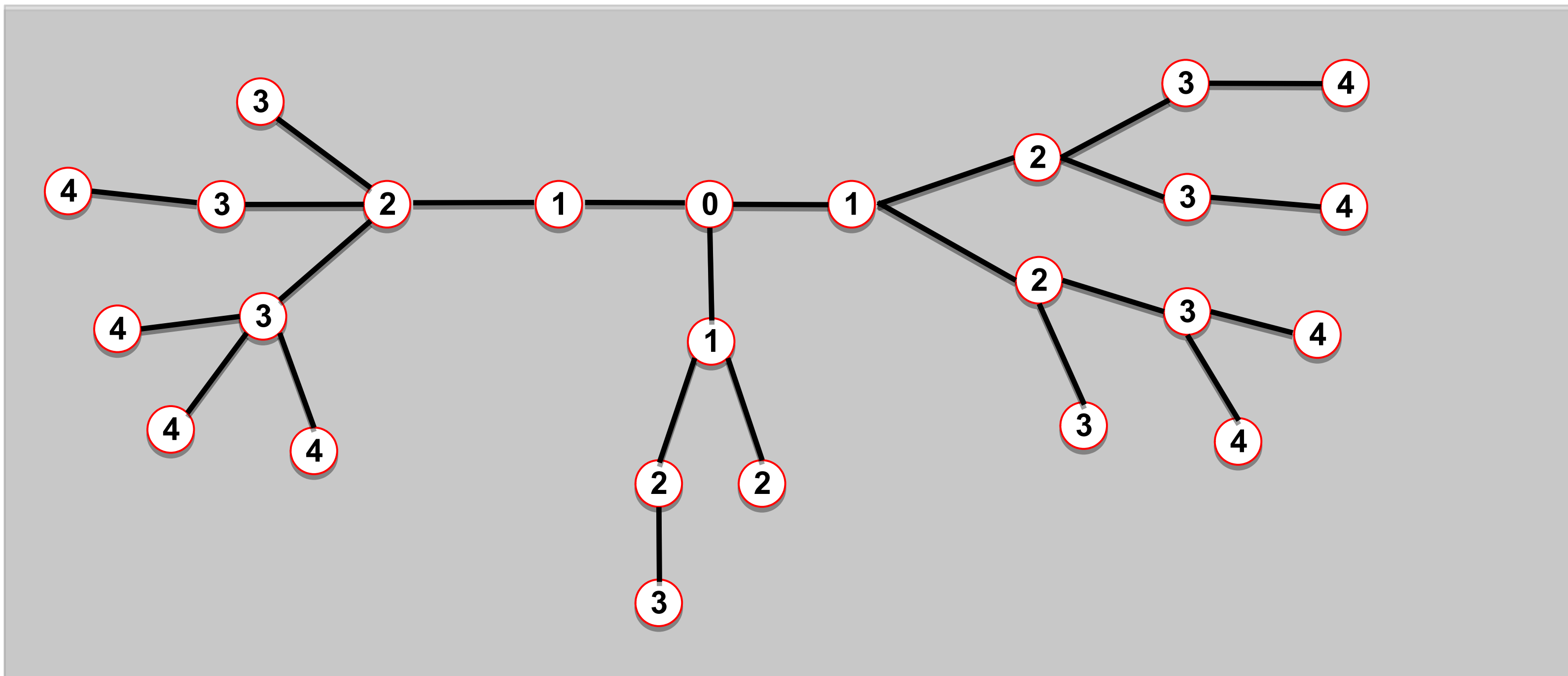
1. Start at 0.
2. Find the nodes adjacent to 0. Mark them as at distance 1. Put them in a queue.
3. Take the first node out of the queue. Find the unmarked nodes adjacent to it in the graph. Mark them with the label of 2. Put them in the queue.



FINDING DISTANCES: BREADTH FIRST SEARCH

Distance between node 0 and node 4:

1. Repeat until you find node 4 or there are no more nodes in the queue.
2. The distance between 0 and 4 is the label of 4 or, if 4 does not have a label, infinity.



NETWORK DIAMETER AND AVERAGE DISTANCE

Diameter: $\boldsymbol{d_{max}}$ the maximum distance between any pair of nodes in the graph.

Average path length/distance, <d>, for a connected graph:

$$\langle d \rangle \equiv \frac{1}{2L_{\max}} \sum_{i,j \neq i} d_{ij}$$

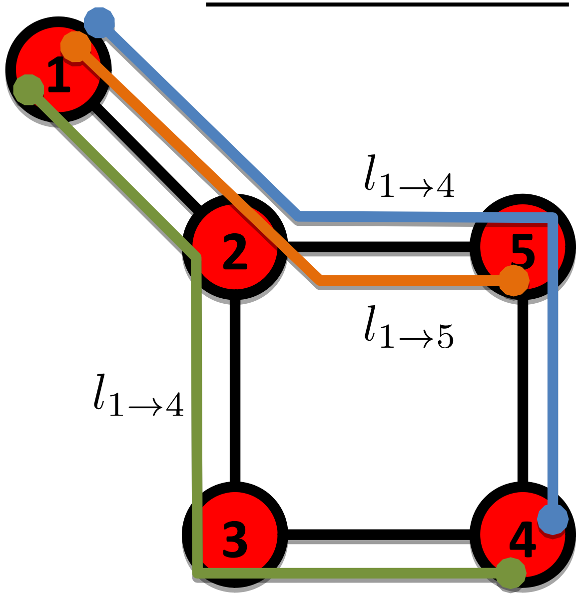
where d_{ij} is the distance from node *i* to node j

In an *undirected graph* $d_{ij} = d_{ji}$, *so* we only need to count them once:

$$\langle d \rangle \equiv \frac{1}{L_{\max}} \sum_{i,j>i} d_{ij}$$

PATHOLOGY: summary

Shortest Path



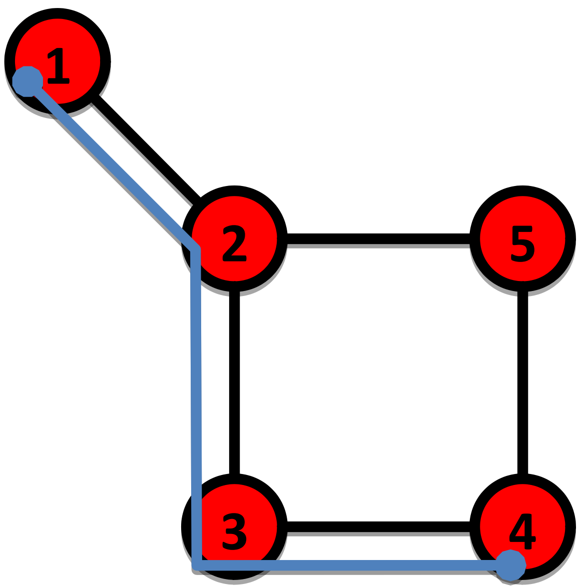
$$l_{1 \to 4} = 3$$

$$l_{1 \to 5} = 2$$

A path with the shortest length between two nodes (distance).

PATHOLOGY: summary

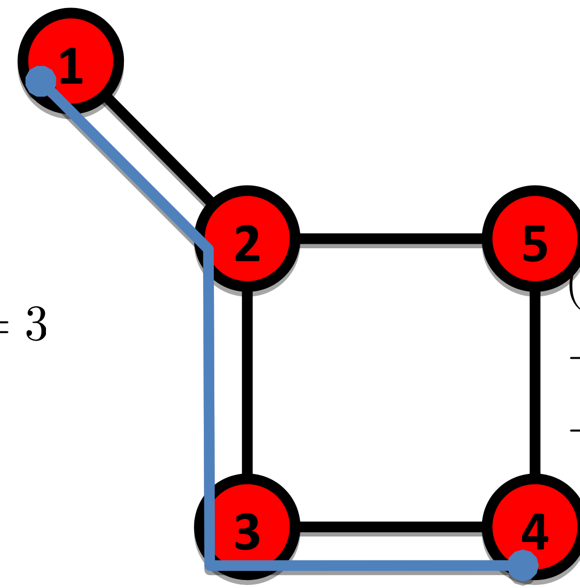
Diameter



$$l_{1\to 4} = 3$$

The length of a longest shortest path in a graph

Average Path Length

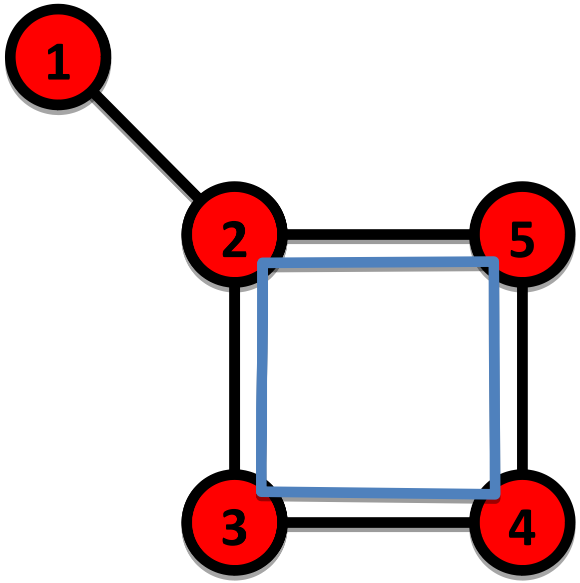


$$\left(l_{1\to 2} + l_{1\to 3} + l_{1\to 4} + l_{1\to 5} + l_{2\to 3} + l_{2\to 4} + l_{2\to 5} + l_{3\to 4} + l_{3\to 5} + l_{4\to 5}\right)/10 = 1.6$$

The average length of the shortest paths for all pairs of nodes.

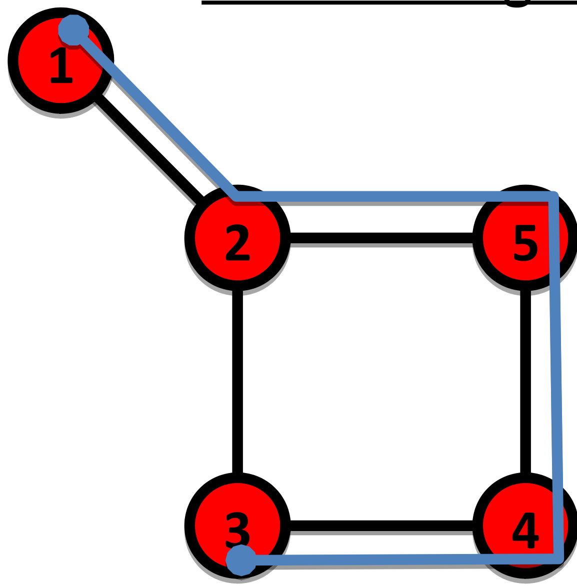
PATHOLOGY: summary

<u>Cycle</u>



A path with the same start and end node.

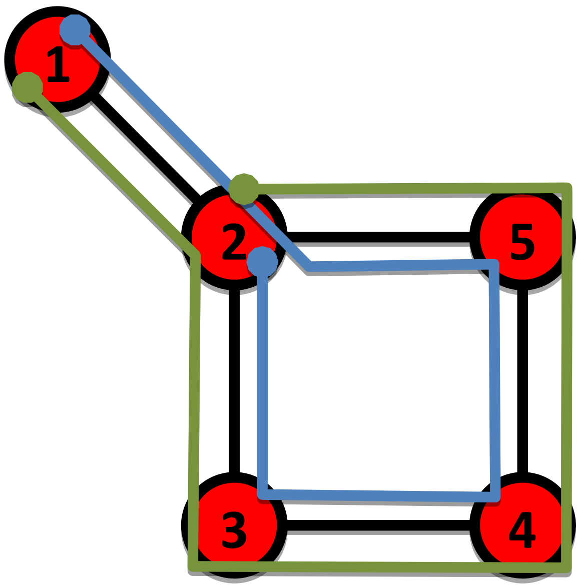
<u>Self-avoiding Path</u>



A path that does not intersect itself.

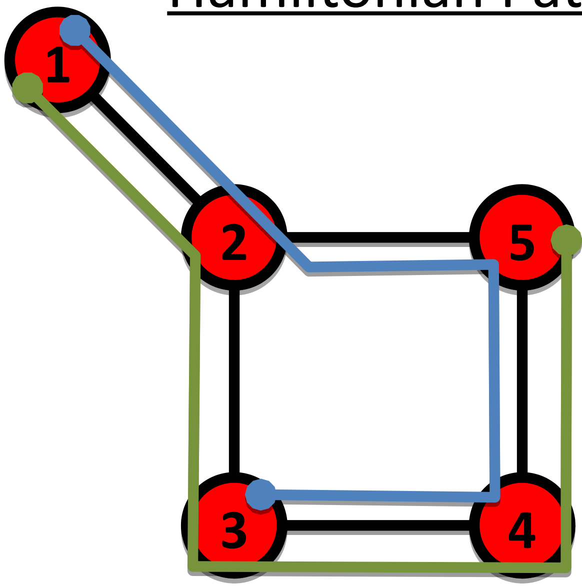
PATHOLOGY: summary

Eulerian Path



A path that traverses each link exactly once.

Hamiltonian Path

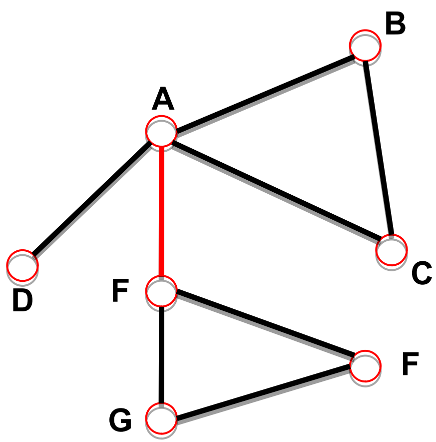


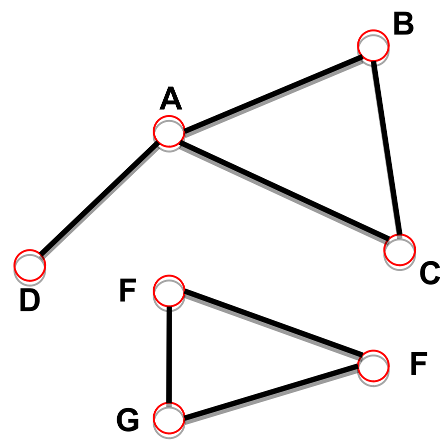
A path that visits each node exactly once.

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.





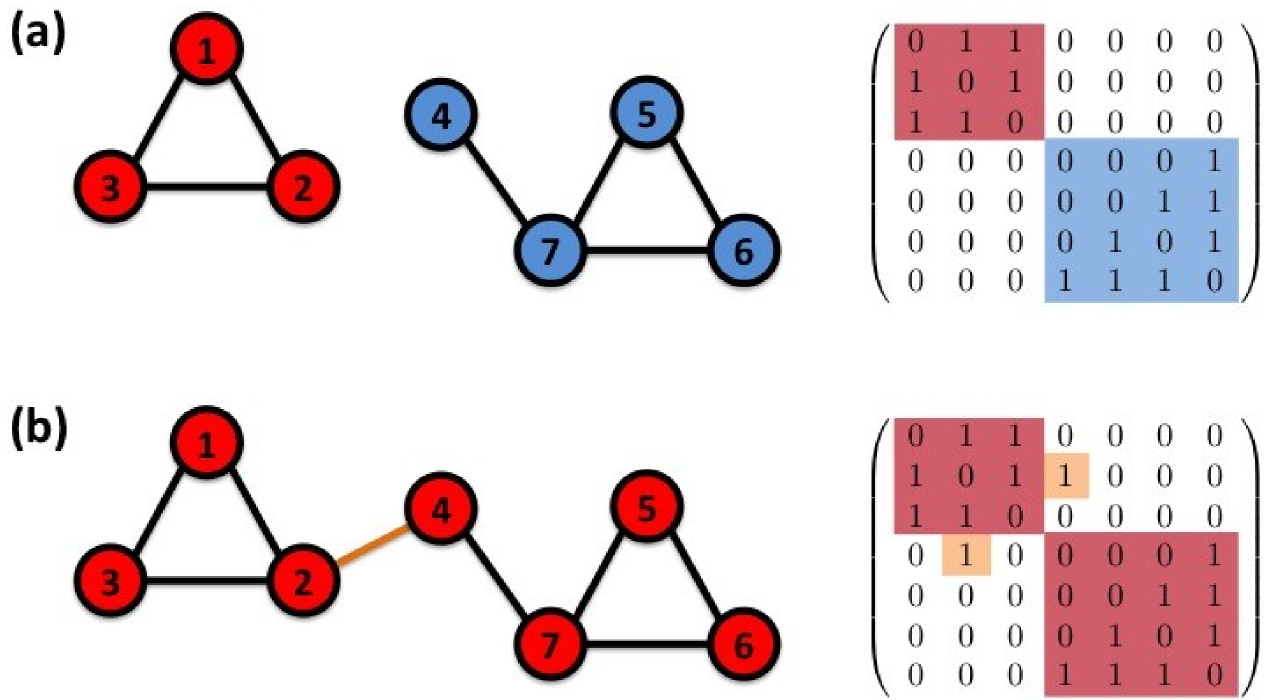
Largest Component:
Giant Component

The rest: **Isolates**

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

CONNECTIVITY OF UNDIRECTED GRAPHS | Adjacency Matrix

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

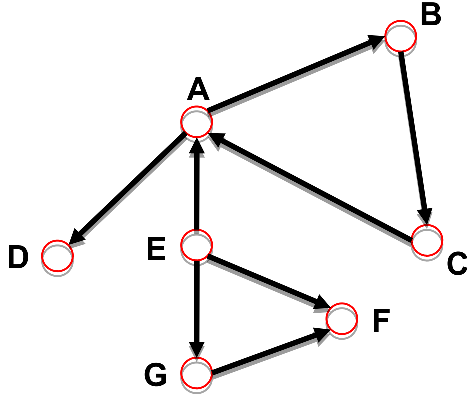


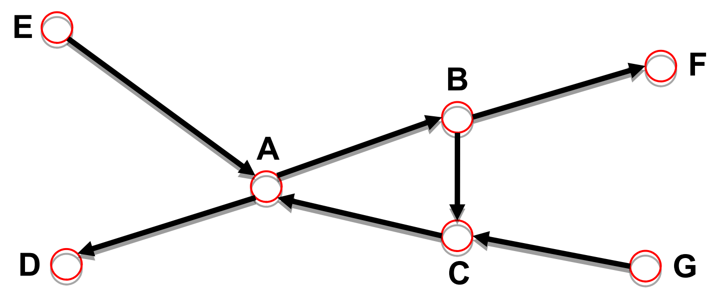
CONNECTIVITY OF DIRECTED GRAPHS

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.

3. Increase the label $n \rightarrow n + 1$. 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.

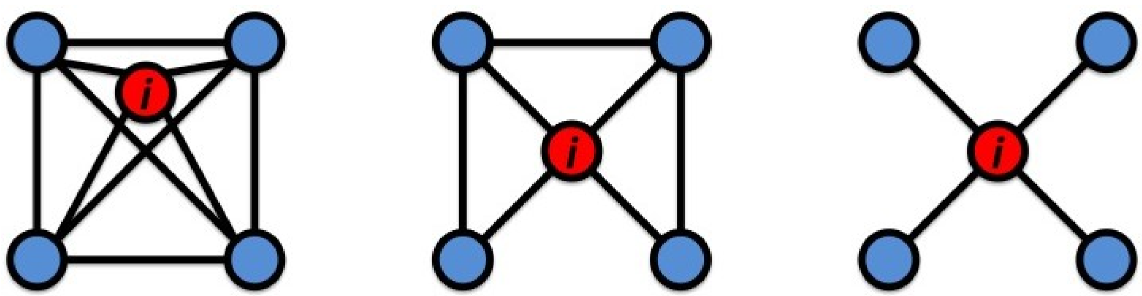
Clustering coefficient

* Clustering coefficient:

what fraction of your neighbors are connected?

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

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



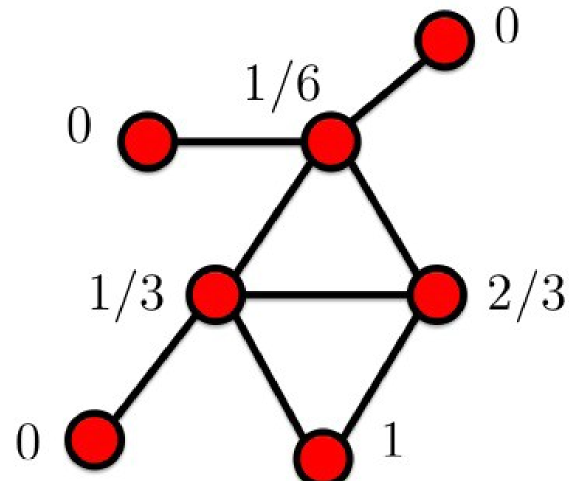
$C_i = 1$ $\quad$ $C_i = 1/2$ $\quad$ $C_i = 0$

Watts & Strogatz, Nature 1998.

Clustering coefficient:

what fraction of your neighbors are connected?

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



$$\langle C \rangle = \frac{13}{42} \approx 0.310$$

$$C = \frac{3}{8} = 0.375$$

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

Watts & Strogatz, Nature 1998.

summary

THREE CENTRAL QUANTITIES IN NETWORK SCIENCE

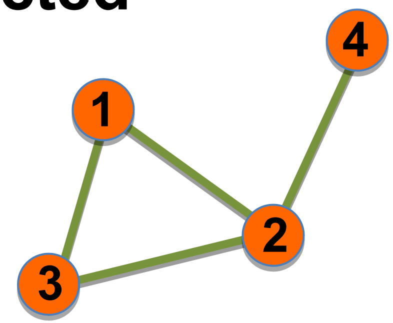
Degree distribution: **P(k)**

Path length: **<*d*>**

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

GRAPHOLOGY 1

Undirected



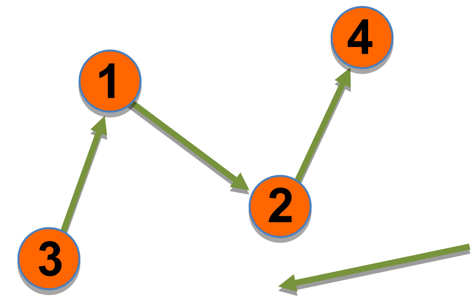
$$A_{ij} = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

$$A_{ii} = 0 \qquad A_{ij} = A_{ji}$$

$$L = \frac{1}{2} \sum_{i,j=1}^{N} A_{ij} \qquad < k > = \frac{2L}{N}$$

Actor network, protein-protein interactions

Directed



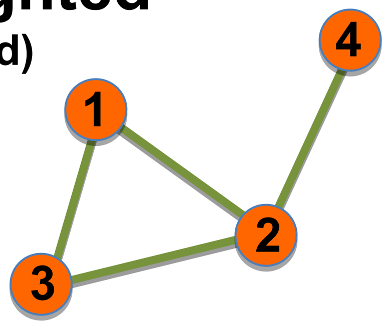
$$A_{ij} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$A_{ii} = 0 \qquad A_{ij} \neq A_{ji}$$

$$L = \sum_{i,j=1}^{N} A_{ij} \qquad < k > = \frac{L}{N}$$

WWW, citation networks

Unweighted
(undirected)



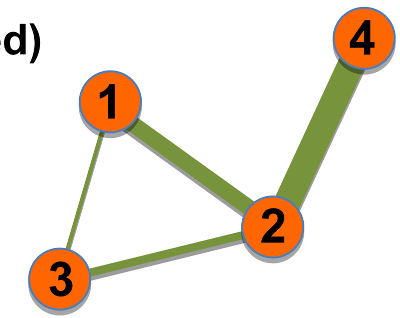
$$A_{ij} = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

$$A_{ii} = 0 \qquad A_{ij} = A_{ji}$$

$$L = \frac{1}{2}\sum_{i,j=1}^{N} A_{ij} \qquad < k >= \frac{2L}{N}$$

protein-protein interactions, www

Weighted
(undirected)



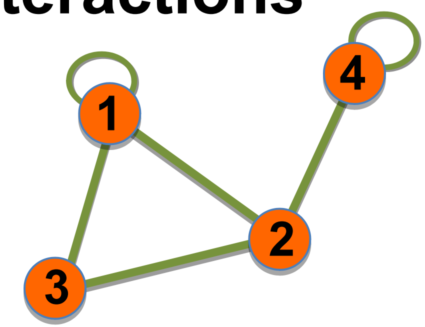
$$A_{ij} = \begin{pmatrix} 0 & 2 & 0.5 & 0 \\ 2 & 0 & 1 & 4 \\ 0.5 & 1 & 0 & 0 \\ 0 & 4 & 0 & 0 \end{pmatrix}$$

$$A_{ii} = 0 \qquad A_{ij} = A_{ji}$$

$$L = \frac{1}{2}\sum_{i,j=1}^{N} nonzero(A_{ij}) \qquad < k >= \frac{2L}{N}$$

Call Graph, metabolic networks

Self-interactions



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

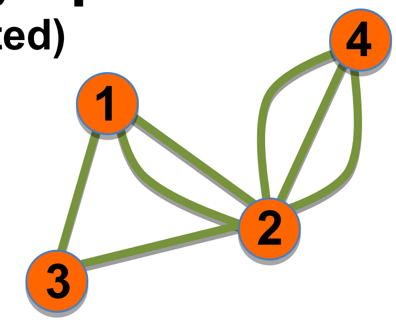
$$A_{ii} \neq 0 \qquad A_{ij} = A_{ji}$$

$$L = \frac{1}{2} \sum_{i,j=1,i\neq j}^{N} A_{ij} + \sum_{i=1}^{N} A_{ii} \qquad ?$$

Protein interaction network, www

Multigraph

(undirected)



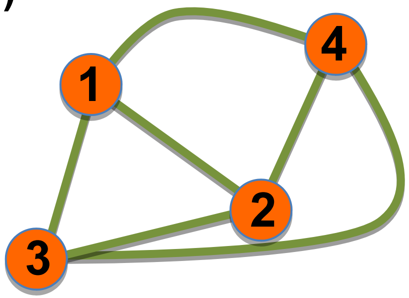
$$A_{ij} = \begin{pmatrix} 0 & 2 & 1 & 0 \\ 2 & 0 & 1 & 3 \\ 1 & 1 & 0 & 0 \\ 0 & 3 & 0 & 0 \end{pmatrix}$$

$$A_{ii} = 0 \qquad A_{ij} = A_{ji}$$

$$L = \frac{1}{2} \sum_{i,j=1}^{N} nonzero(A_{ij}) \qquad <k>= \frac{2L}{N}$$

Social networks, collaboration networks

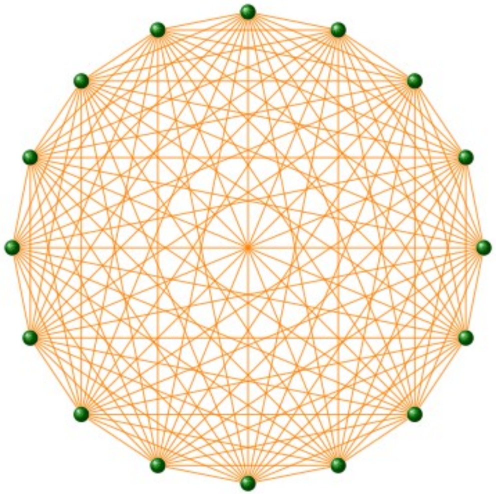
Complete Graph
(undirected)



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

$$A_{ii} = 0 \qquad A_{i \neq j} = 1$$

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



GRAPHOLOGY: Real networks can have multiple characteristics

WWW > **d**irected multigraph with self-interactions

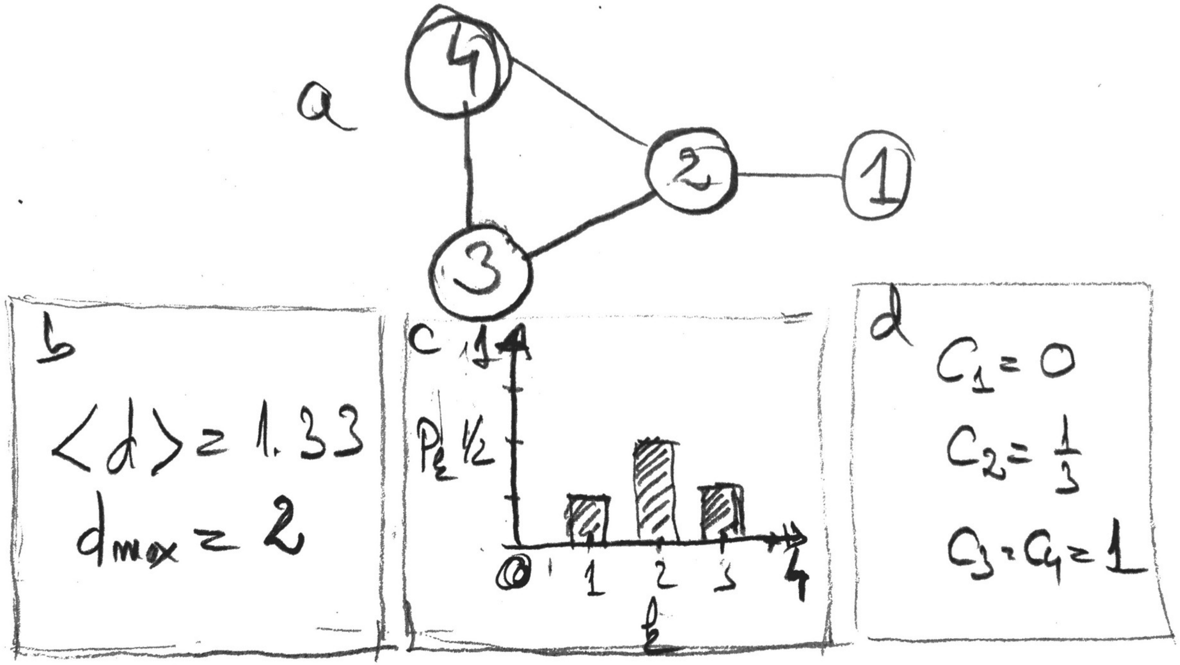
Protein Interactions > **u**ndirected unweighted with self-interactions

Collaboration network > **u**ndirected multigraph or weighted

Mobile phone calls > directed, weighted

Facebook Friendship links > **u**ndirected, unweighted

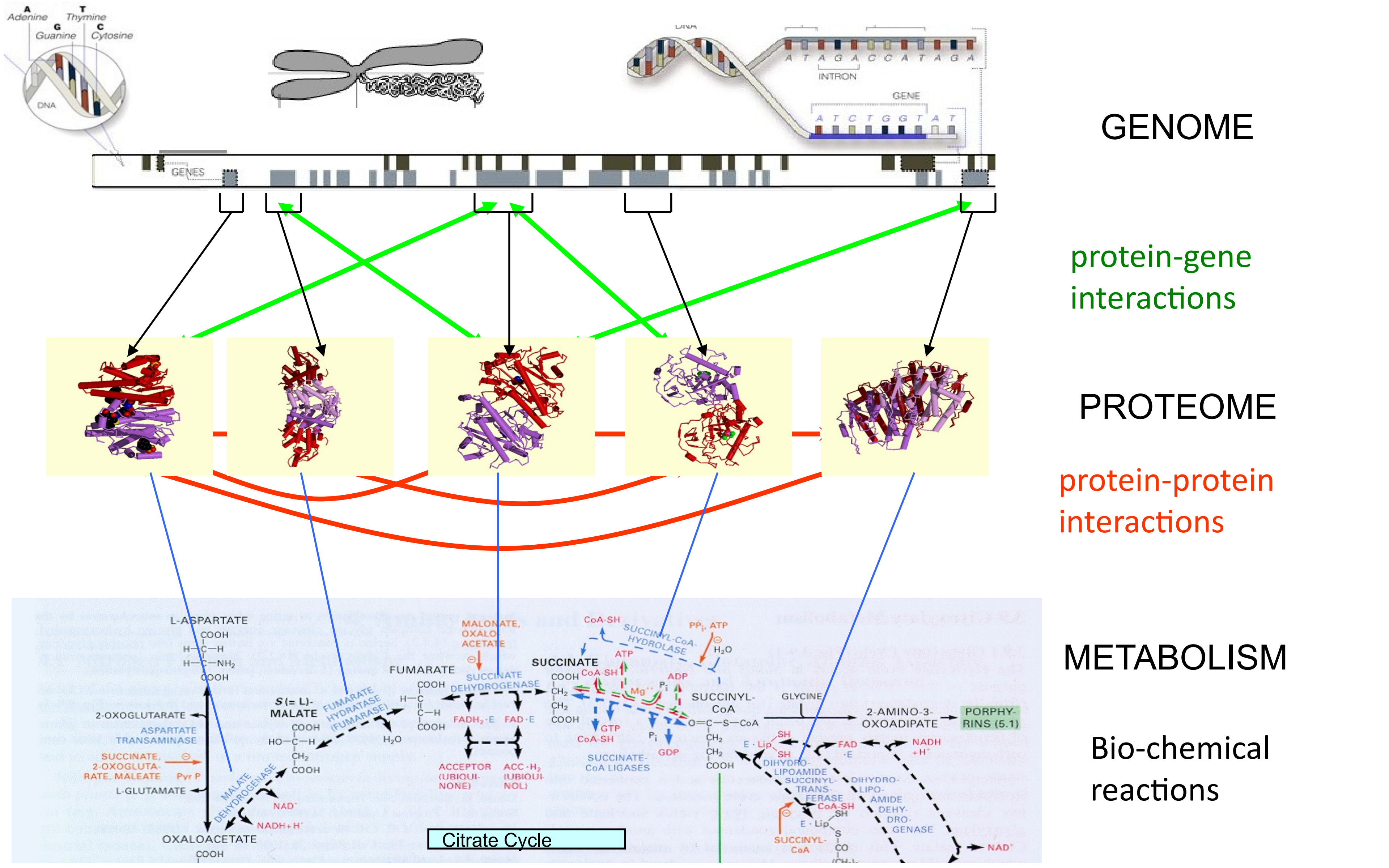
THREE CENTRAL QUANTITIES IN NETWORK SCIENCE



A. Degree distribution: p_k

B. Path length: $\langle d \rangle$

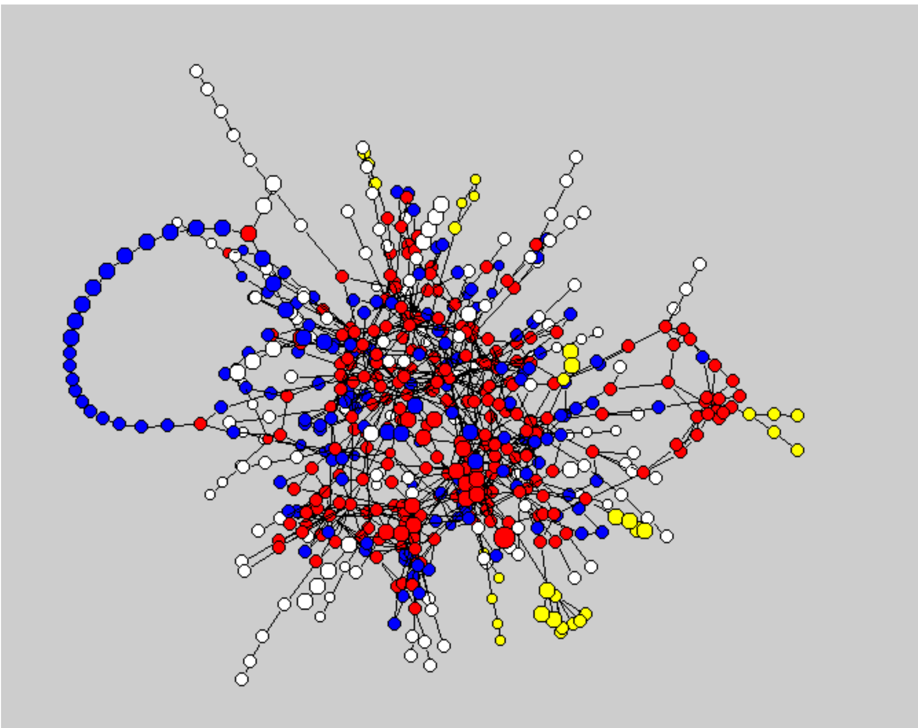
C. Clustering coefficient: $$C_i = \frac{2e_i}{k_i(k_i - 1)}$$

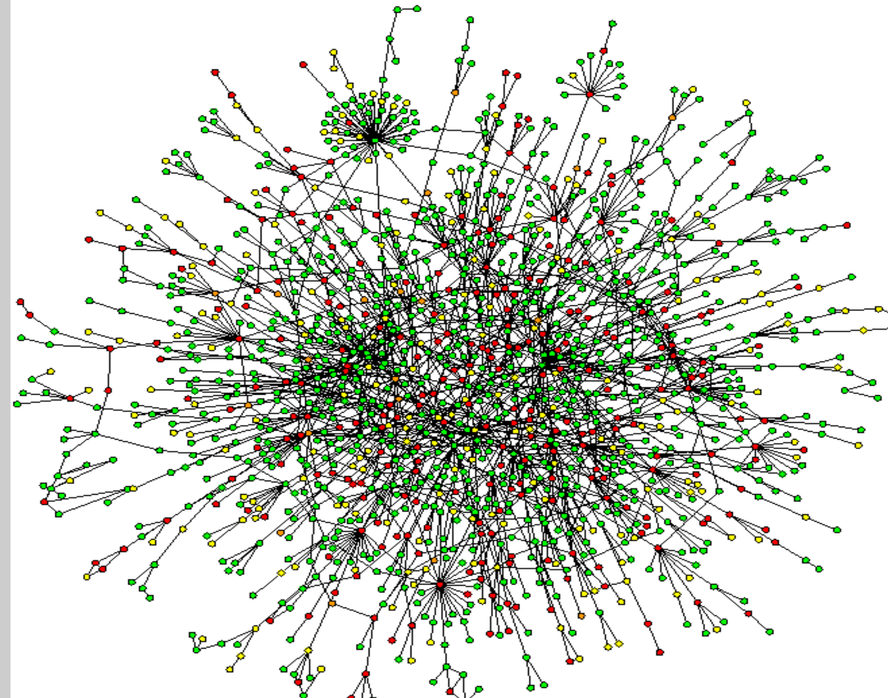


GENOME
protein-gene interactions
PROTEOME
protein-protein interactions
METABOLISM
Bio-chemical reactions
Citrate Cycle

Metabolic Network

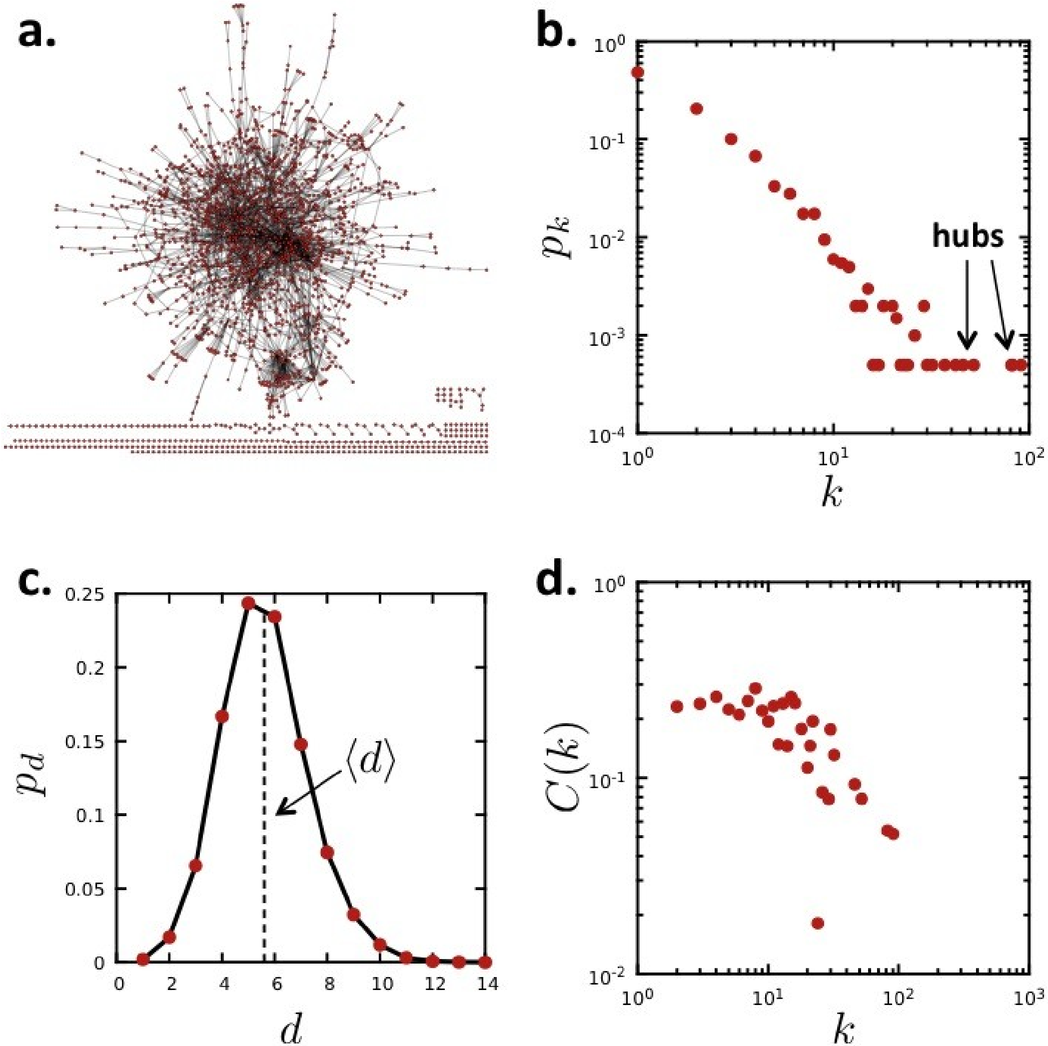
Protein Interactions





A CASE STUDY: PROTEIN-PROTEIN INTERACTION NETWORK

A CASE STUDY: PROTEIN-PROTEIN INTERACTION NETWORK



Undirected network

N=2,018 proteins as nodes

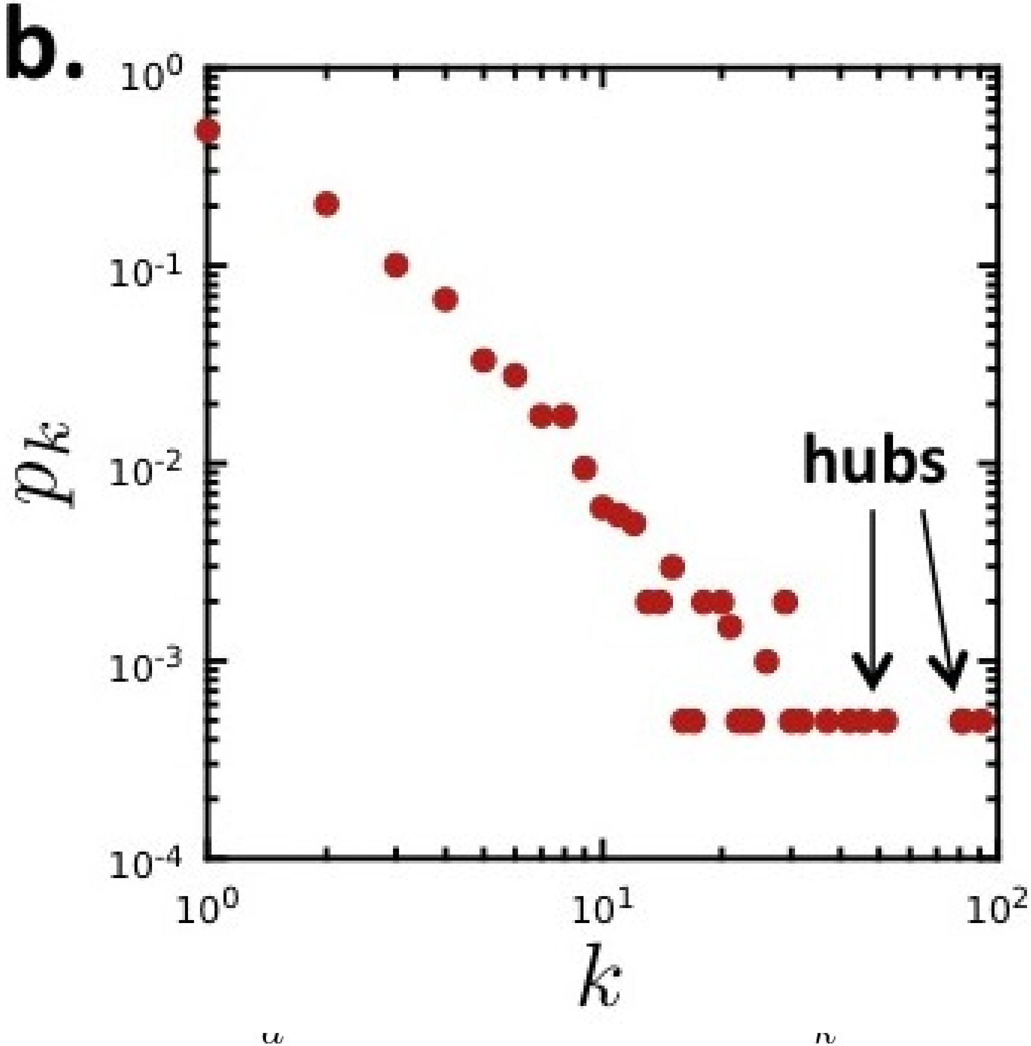
L=2,930 binding interactions as links.

Average degree <k>=2.90.

Not connected: 185 components

the largest (giant component) 1,647 nodes

A CASE STUDY: PROTEIN-PROTEIN INTERACTION NETWORK

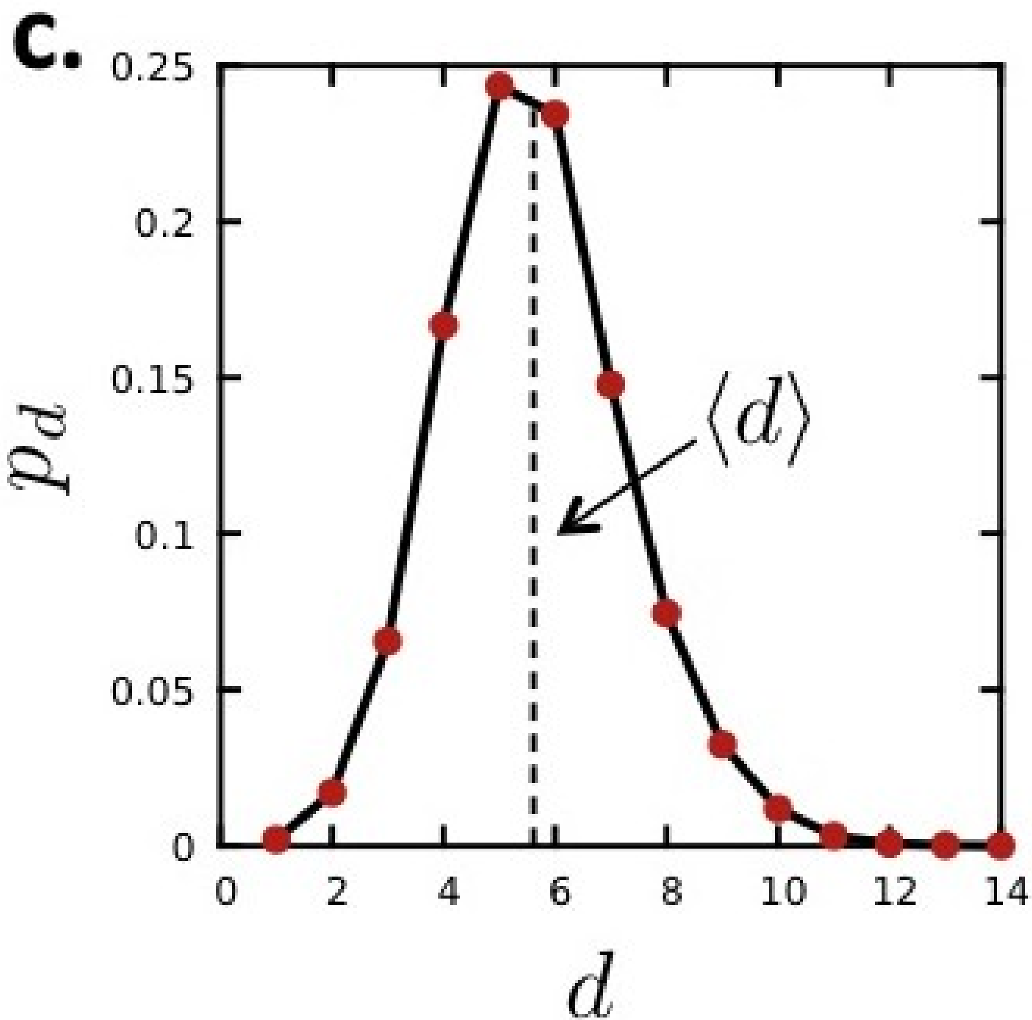


$\mathbf{p_k}$ is the probability that a node has degree **k**.

N_k = # nodes with degree k

$p_k = N_k / N$

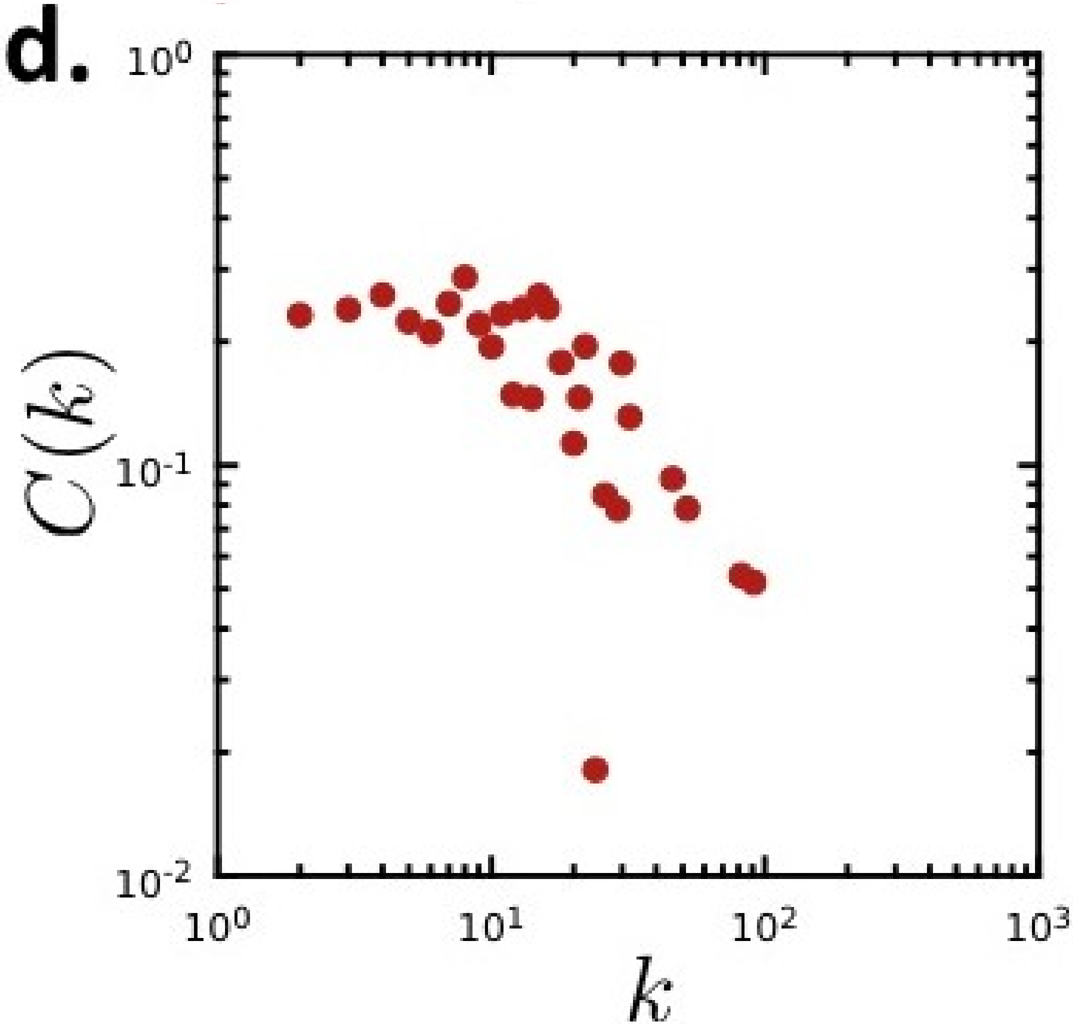
A CASE STUDY: PROTEIN-PROTEIN INTERACTION NETWORK

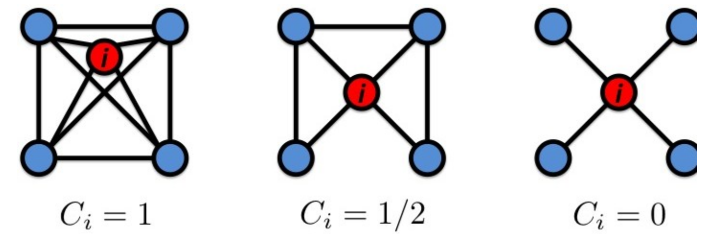


d_{max}=14

<d>=5.61

A CASE STUDY: PROTEIN-PROTEIN INTERACTION NETWORK





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

<C>=0.12