Frontiers of Network Science
Fall 2021

Class 4: Graph Theory II
(Chapter 2 in Textbook)

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based on slides by Albert-László Barabási & Roberta Sinatra

Reference Networks

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

Degree, Average Degree and Degree Distribution

A BIT OF STATISTICS

BRIEF STATISTICS REVIEW

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

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:

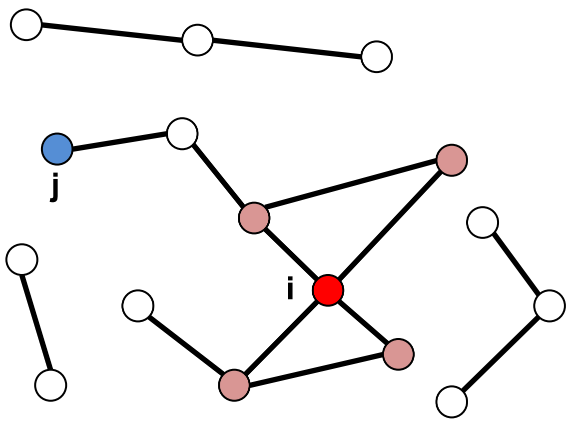
$$p_x = \frac{1}{N}\sum_i \delta_{x,x_i}$$

where p_x follows

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

AVERAGE DEGREE

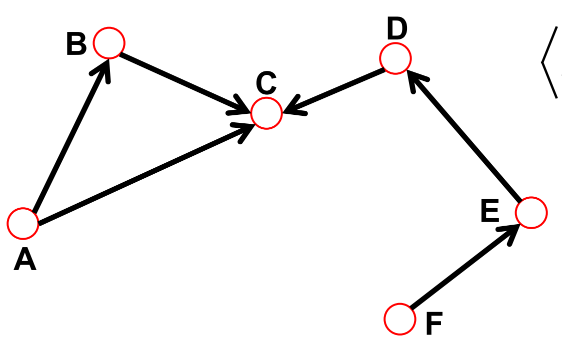
Undirected



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

N – the number of nodes in the graph

Directed

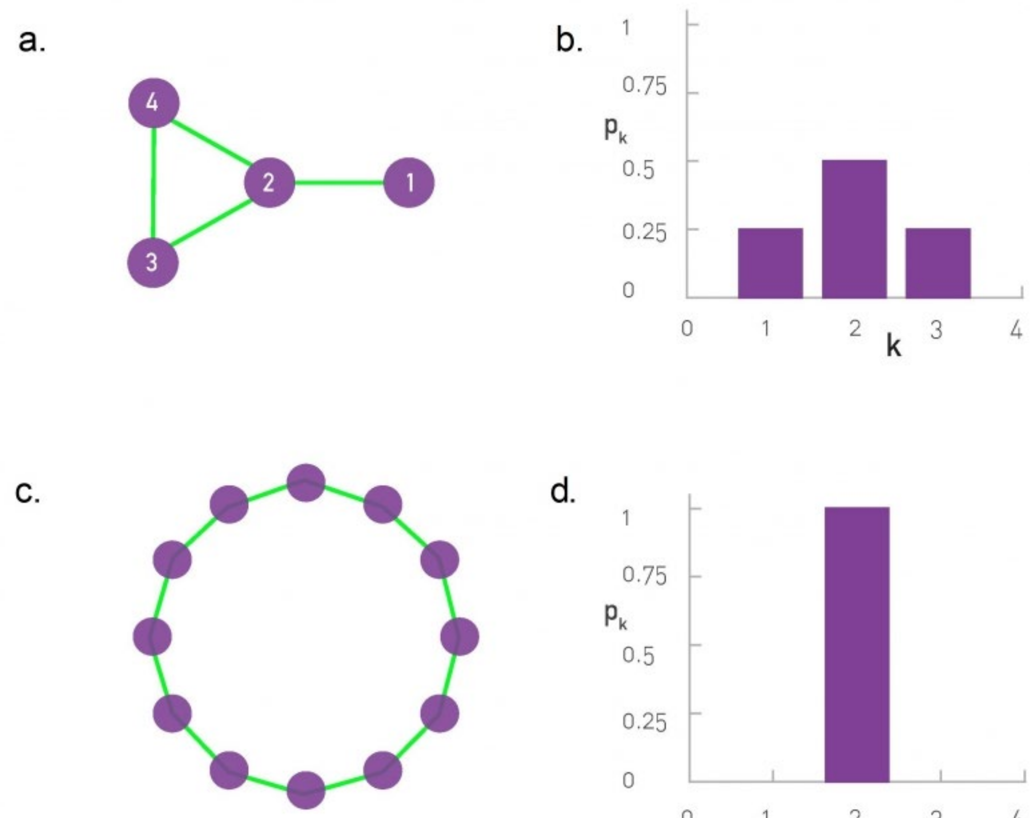


$$\langle k^{in} \rangle \equiv \frac{1}{N}\sum_{i=1}^{N} k_i^{in}, \quad \langle k^{out} \rangle \equiv \frac{1}{N}\sum_{i=1}^{N} k_i^{out}, \quad \langle k^{in} \rangle = \langle k^{out} \rangle$$

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

Degree distribution

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



N_k = # nodes with degree k

$P(k) = N_k / N$ ❾ plot

DEGREE DISTRIBUTION

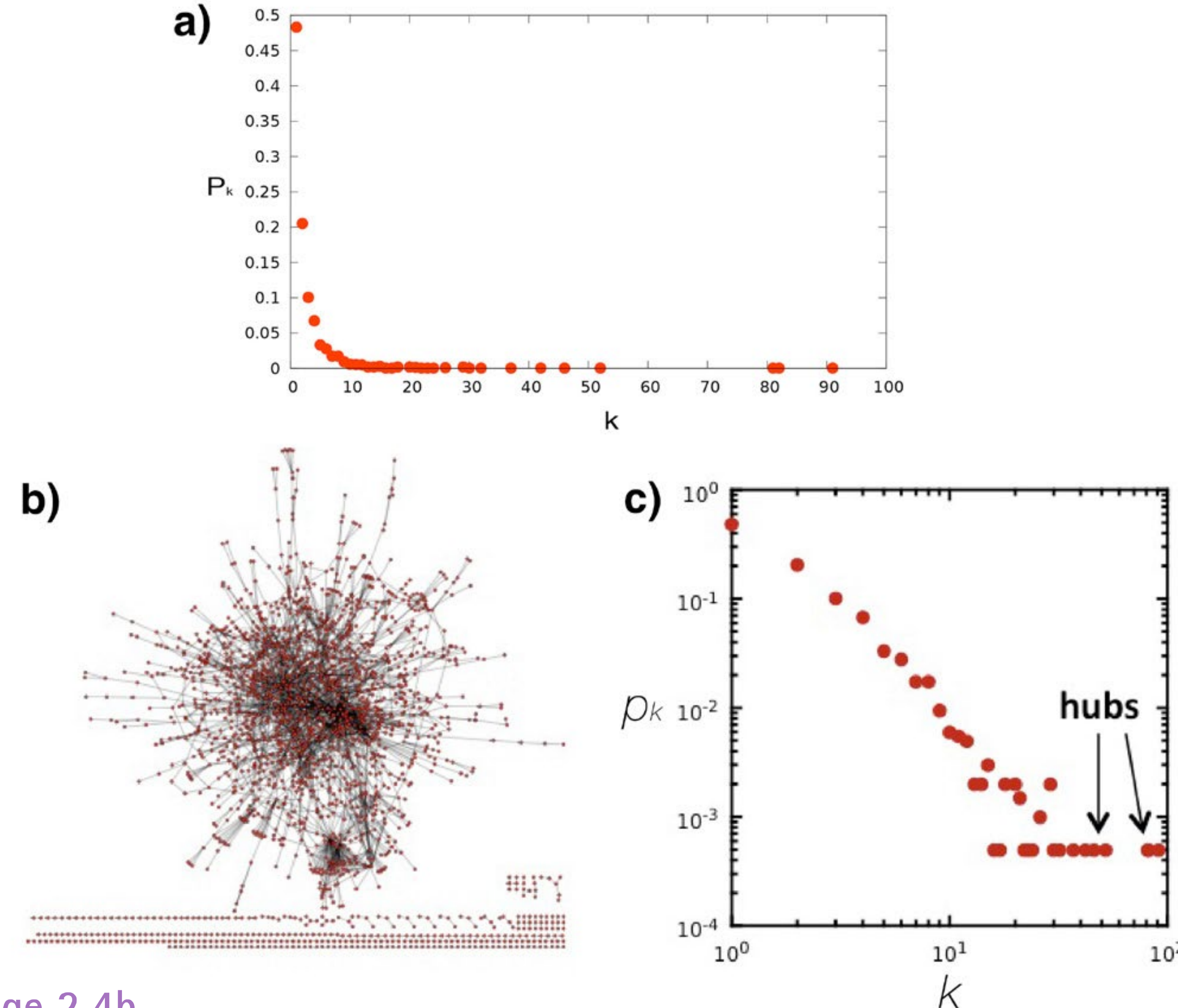


Image 2.4b

DEGREE DISTRIBUTION

Discrete Representation: 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 k_1 and k_2.

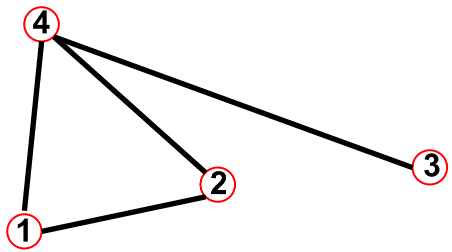
Normalization condition:

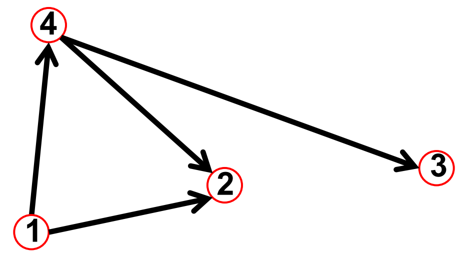
$$\sum_{0}^{\infty} p_k = 1 \qquad \int_{K_{min}}^{\infty} p(k)dk = 1$$

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

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.

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

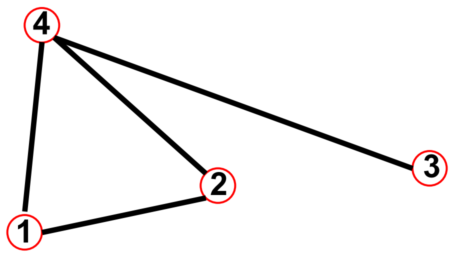
Note that for a directed graph (right) the matrix is not symmetric.

$A_{ij} = 1$ 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



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

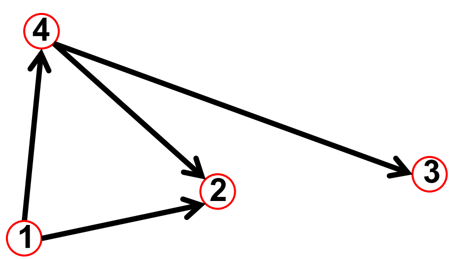
$$A_{ij} = A_{ji}$$
$$A_{ii} = 0$$

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

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

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

Directed



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

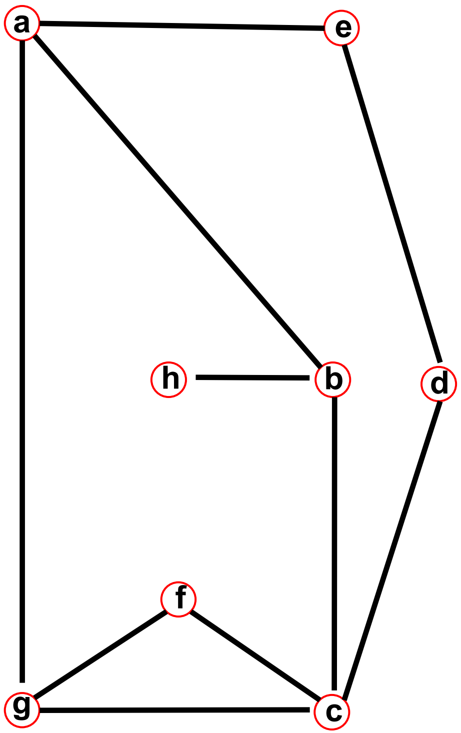
$$A_{ij} \neq A_{ji}$$
$$A_{ii} = 0$$

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

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

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

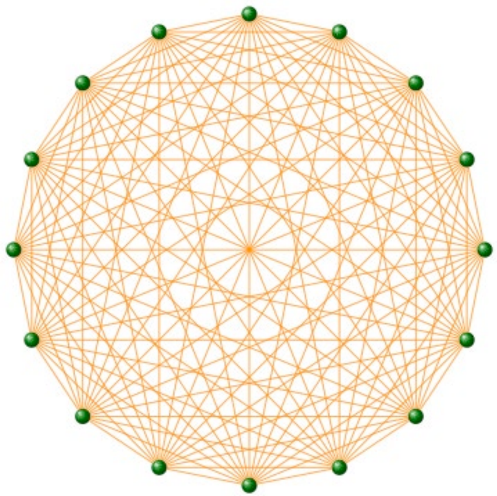
ADJACENCY MATRIX



	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

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:

$$L \ll L_{max}$$

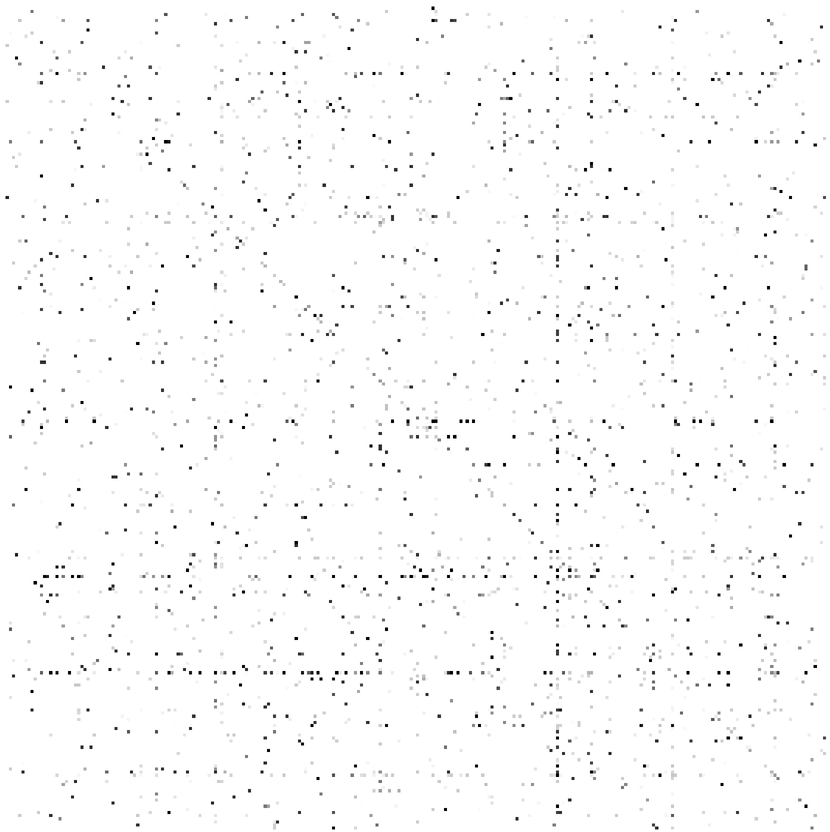
or

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

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



WEIGHTED AND UNWEIGHTED NETWORKS

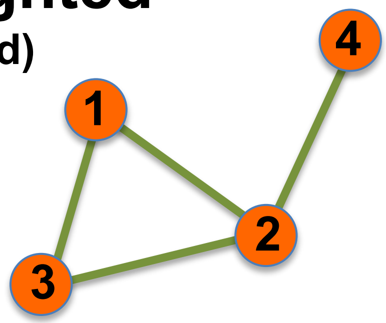
WEIGHTED AND UNWEIGHTED NETWORKS

$$\boldsymbol{A_{ij} = w_{ij}}$$

GRAPHOLOGY 1

Unweighted

(undirected)



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

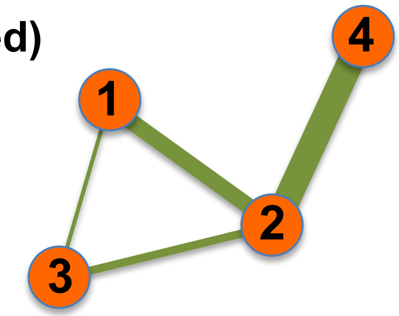
$$A_{ii} = 0 \qquad A_{ij} = A_{ji}$$

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

protein-protein interactions, www

Weighted

(undirected)



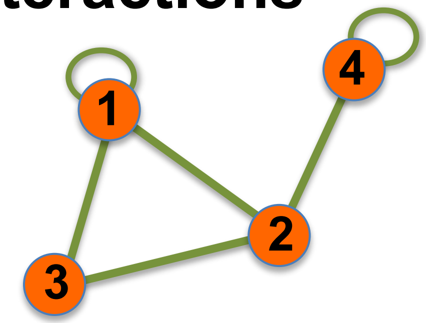
$$A_{ij} = \begin{pmatrix} 0 & 2 & 0.5 & 0 \\ 2 & 0 & 1 & 4 \\ 0.5 & 1 & 0 & 0 \\ 0 & 4 & 0 & 0 \end{pmatrix}$$

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

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

Call Graph, metabolic networks

Self-interactions



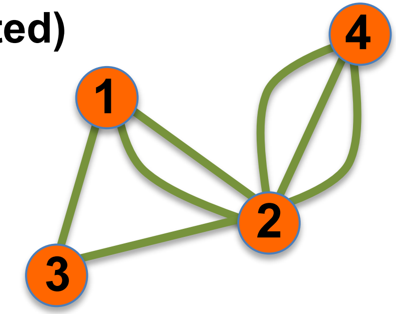
$$A_{ij} = \begin{pmatrix} 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix}$$

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

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

Protein interaction network, www

Multigraph
(undirected)



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

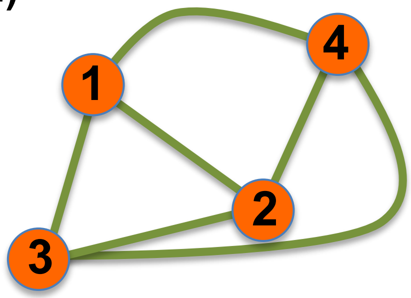
$$A_{ii} = 0 \qquad A_{ij} = A_{ji}$$

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

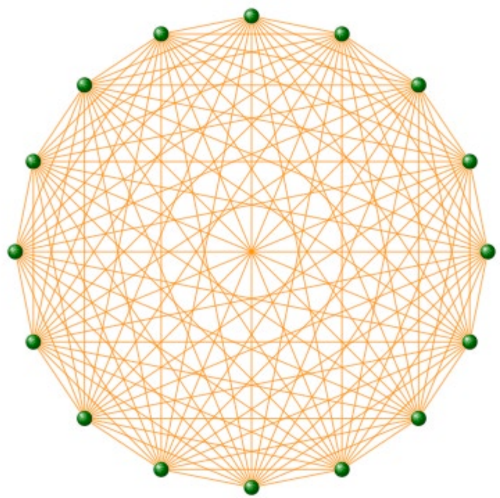
Social networks, collaboration networks

Complete Graph

(undirected)



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

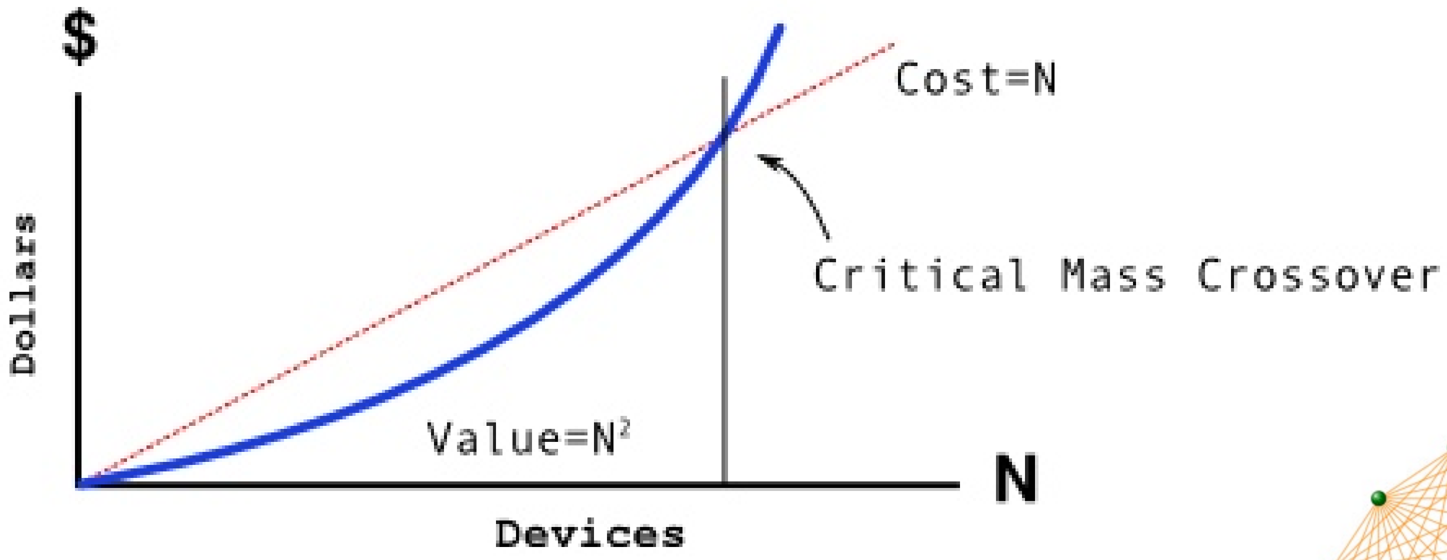


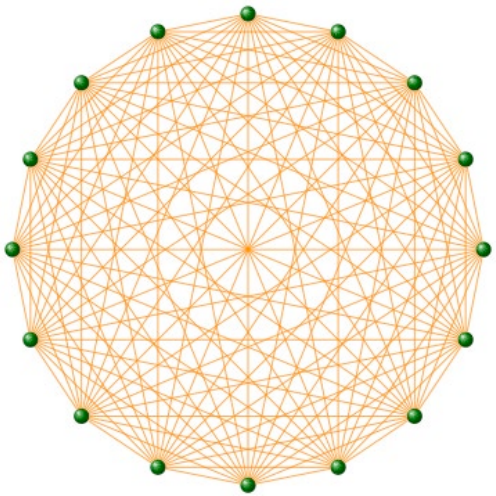
$$A_{ii} = 0 \qquad A_{i \neq j} = 1$$

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

Actor network, protein-protein interactions

METCALFE'S LAW



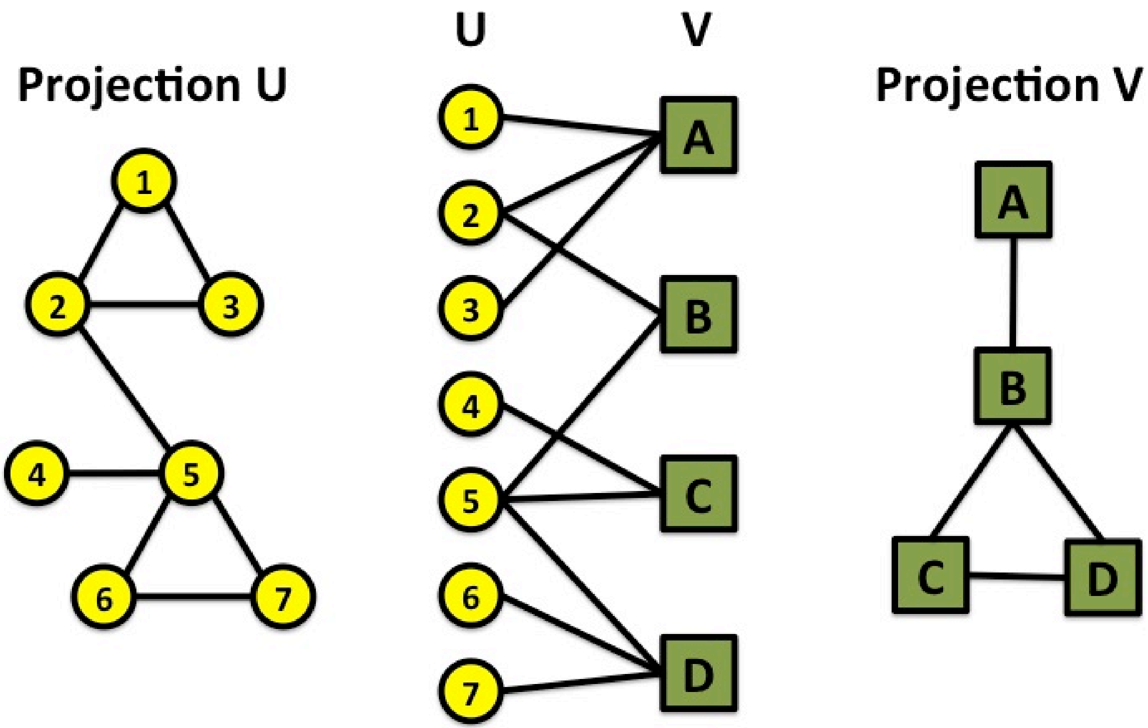


The maximum number of links a network of N nodes can have is: $L_{\max} = \binom{N}{2} = \frac{N(N-1)}{2}$

BIPARTITE NETWORKS

BIPARTITE GRAPHS

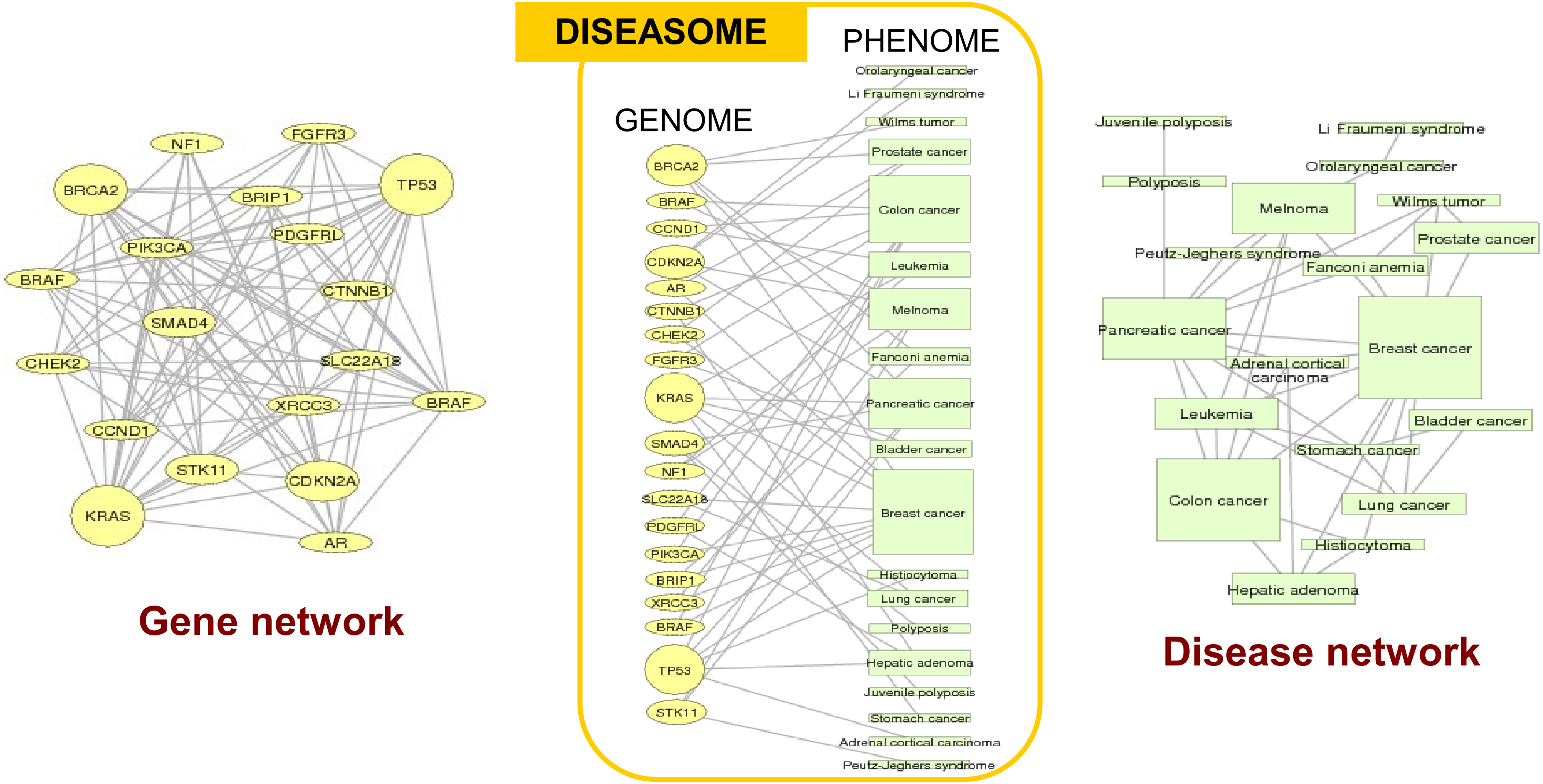
bipartite graph (or **bigraph**) is a graph whose nodes can be divided into two disjoint sets *U* and *V* such that every link connects a node in *U* to one in *V*; that is, *U* and *V* are independent sets.



Examples:

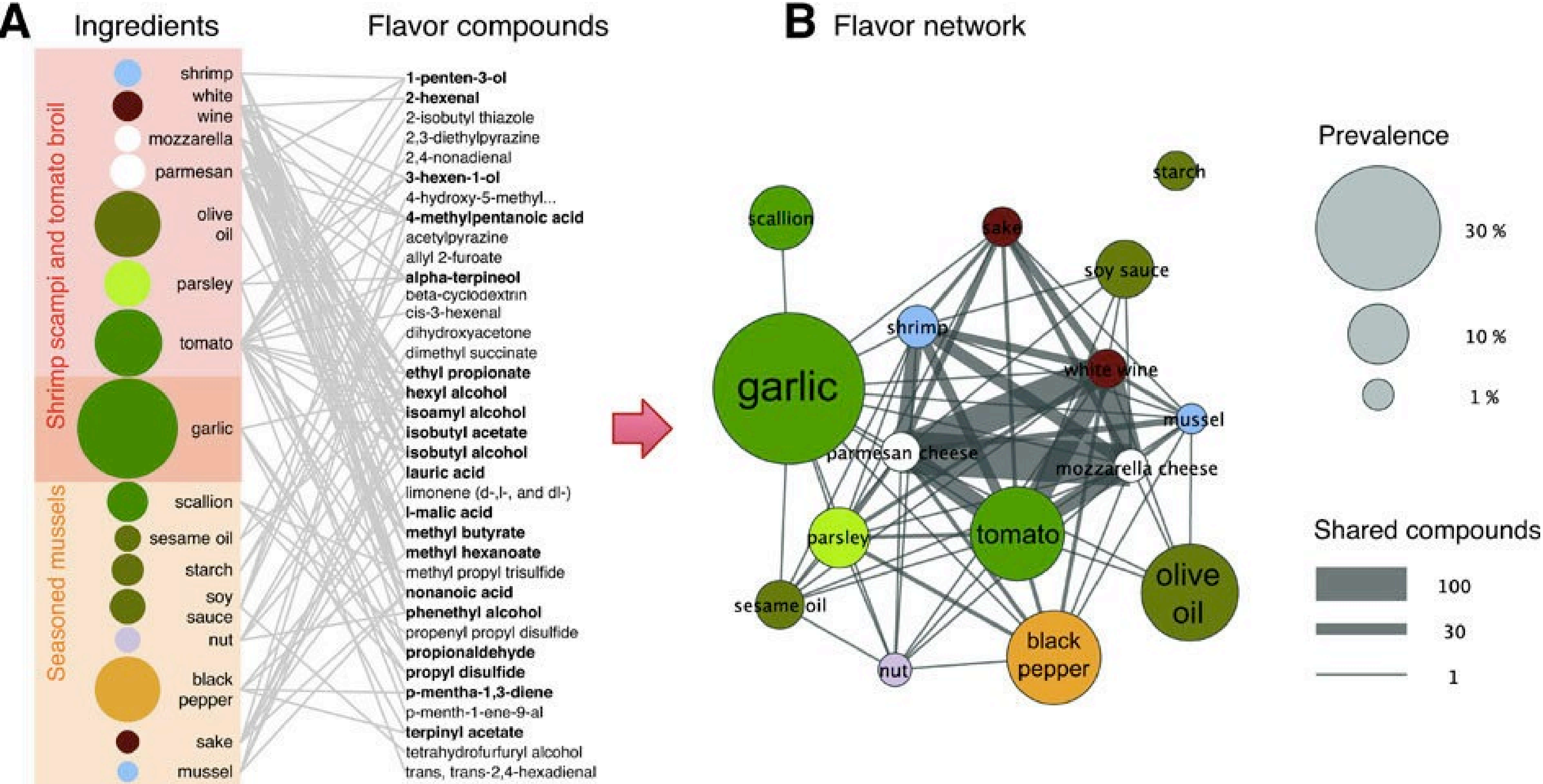
Hollywood actor network
Collaboration networks
Disease network (diseasome)

GENE NETWORK – DISEASE NETWORK

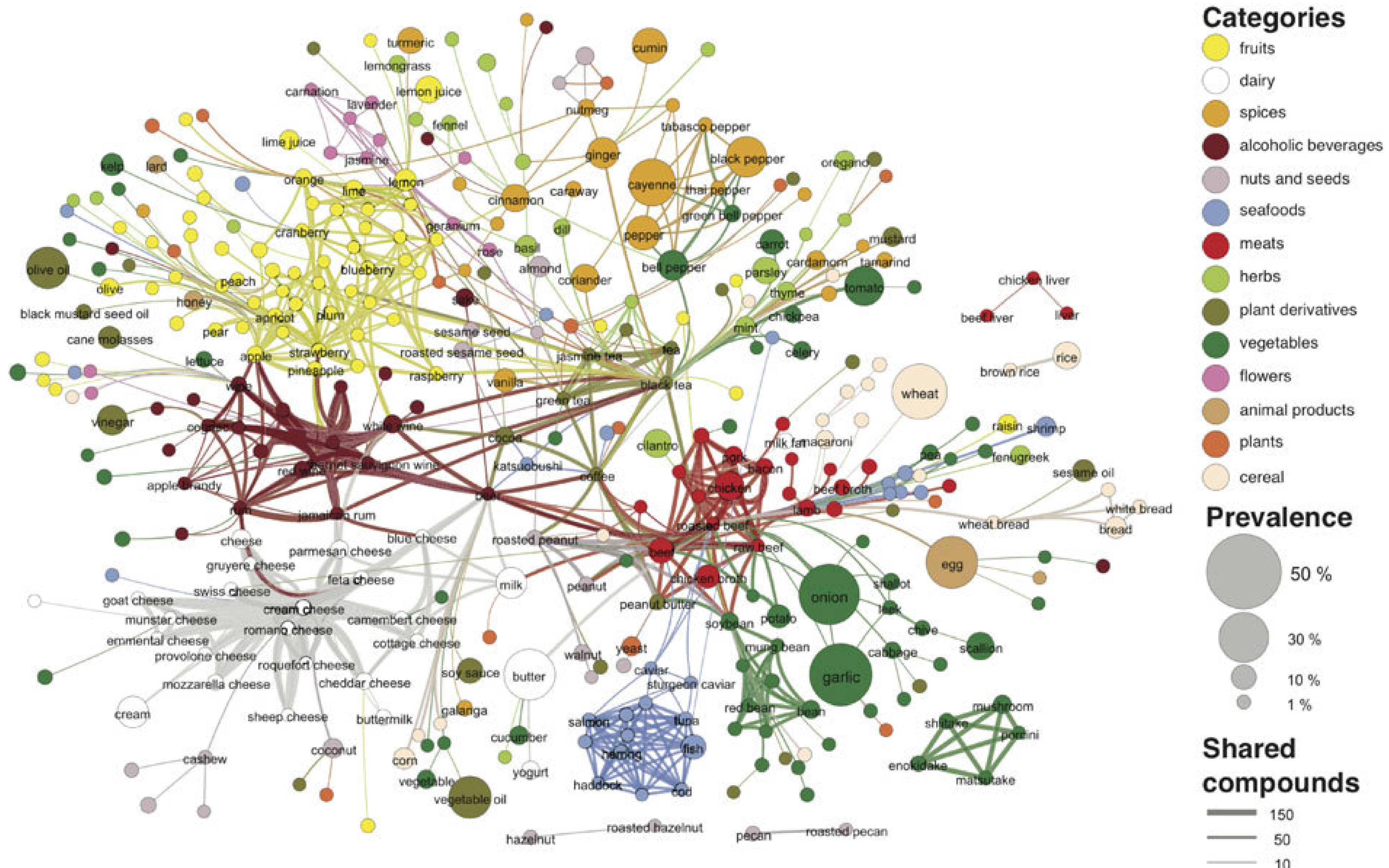


Goh, Cusick, Valle, Childs, Vidal & Barabási, PNAS (2007)

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).



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

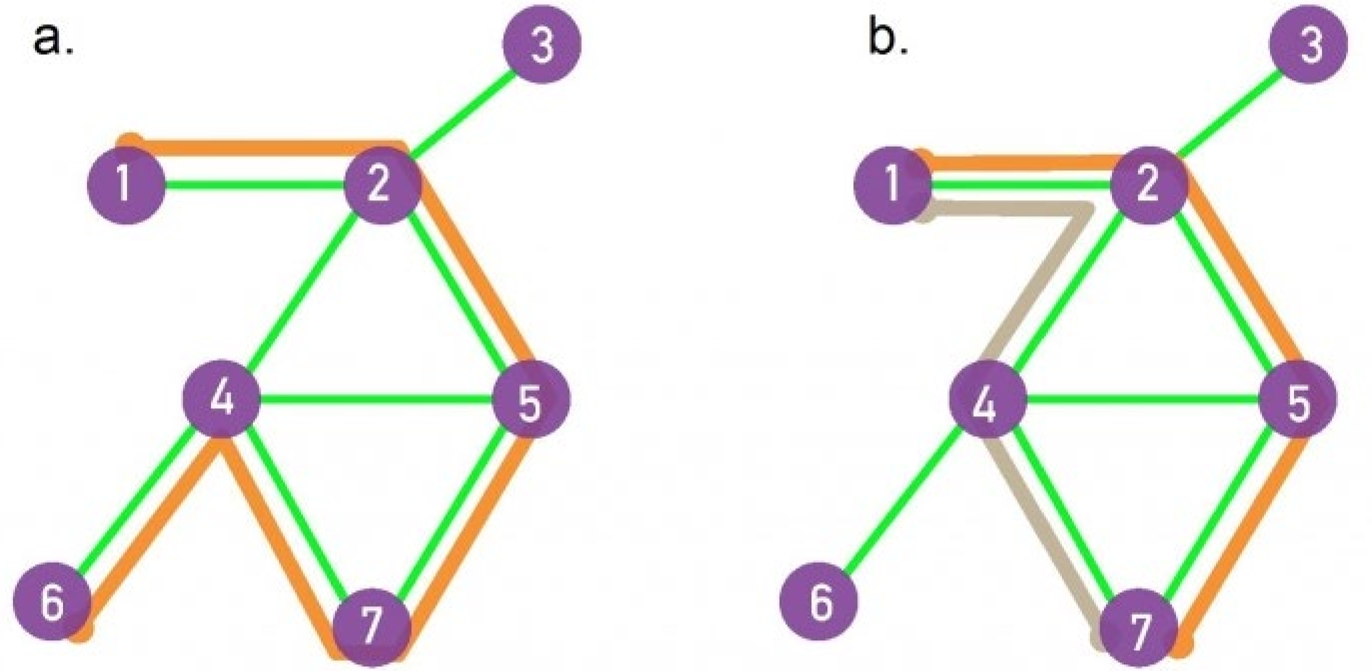
PATHOLOGY

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

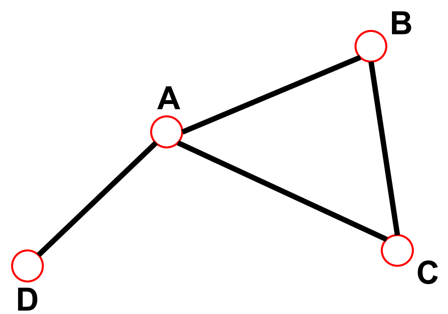
$$P_n = \{i_0, i_1, i_2, \dots, i_n\} \qquad P_n = \{(i_0, i_1), (i_1, i_2), (i_2, i_3), \dots, (i_{n-1}, i_n)\}$$



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

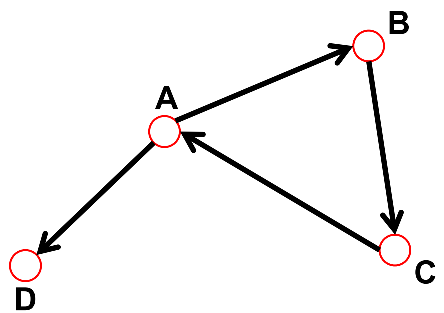
DISTANCE IN A GRAPH

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 BCA path).

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

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

Length n=2: 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:

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

Length n: 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*

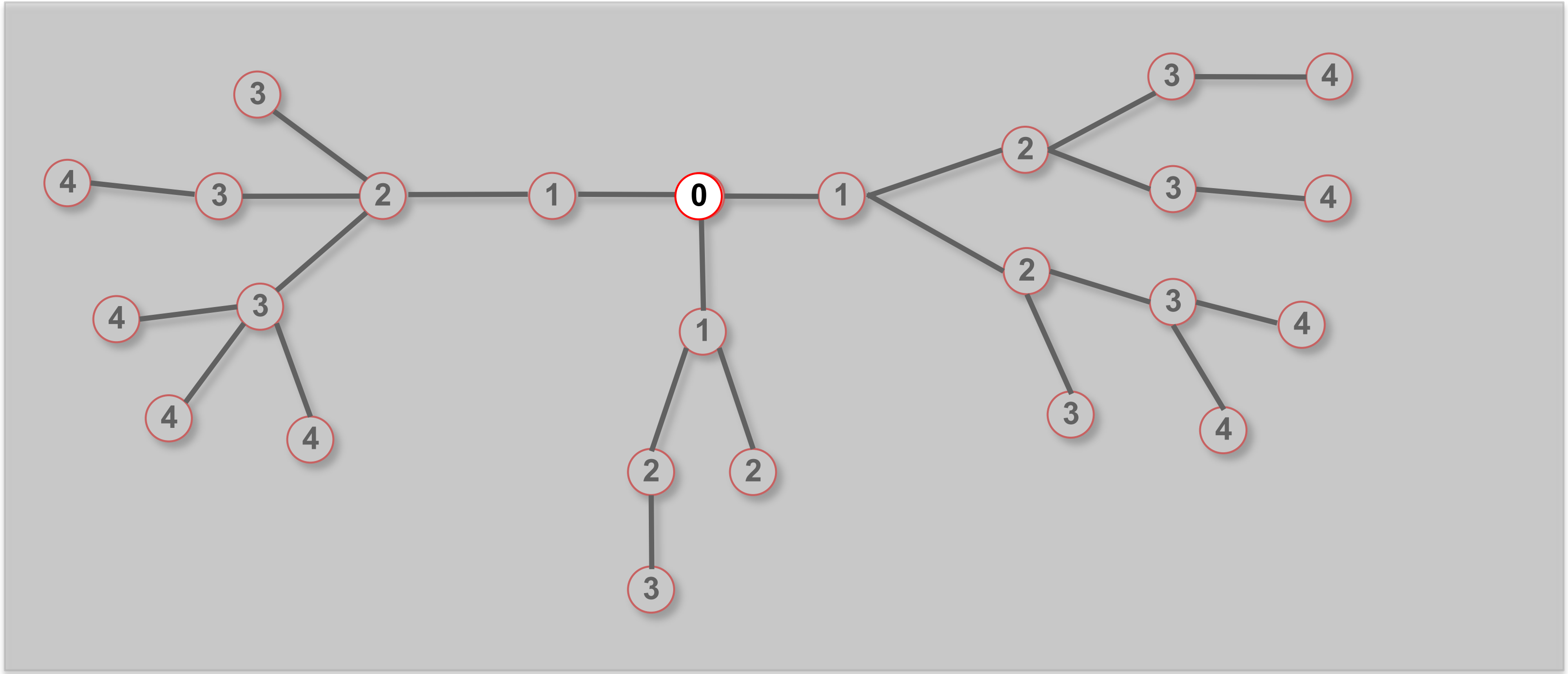
$$N_{ij}^{(n)} = [A^n]_{ij}$$

**holds for both directed and undirected networks.*

FINDING DISTANCES: BREADTH FIRST SEARCH

Distance between node 0 and node 4:

1.Start at 0.

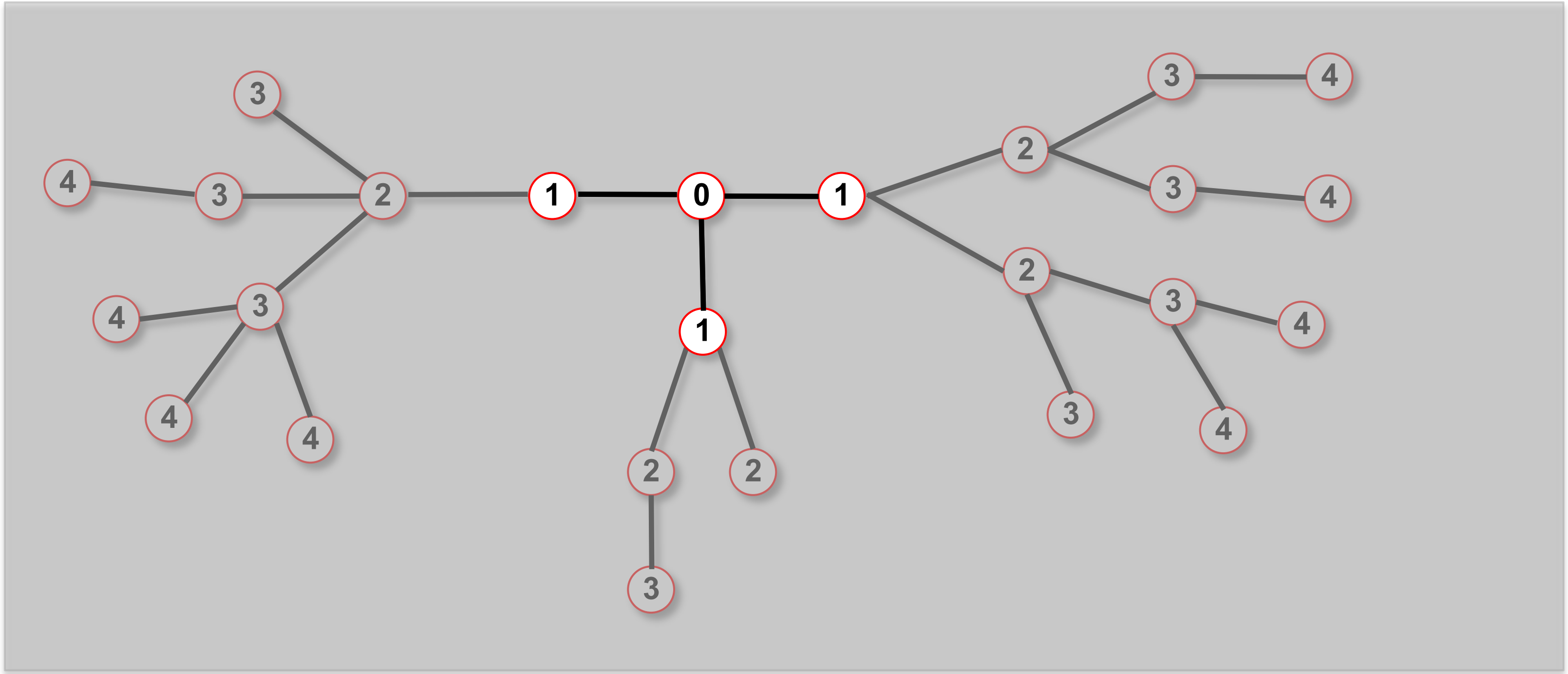


FINDING DISTANCES: BREADTH FIRST SEARCH

Distance between node 0 and node 4:

1.Start at 0.

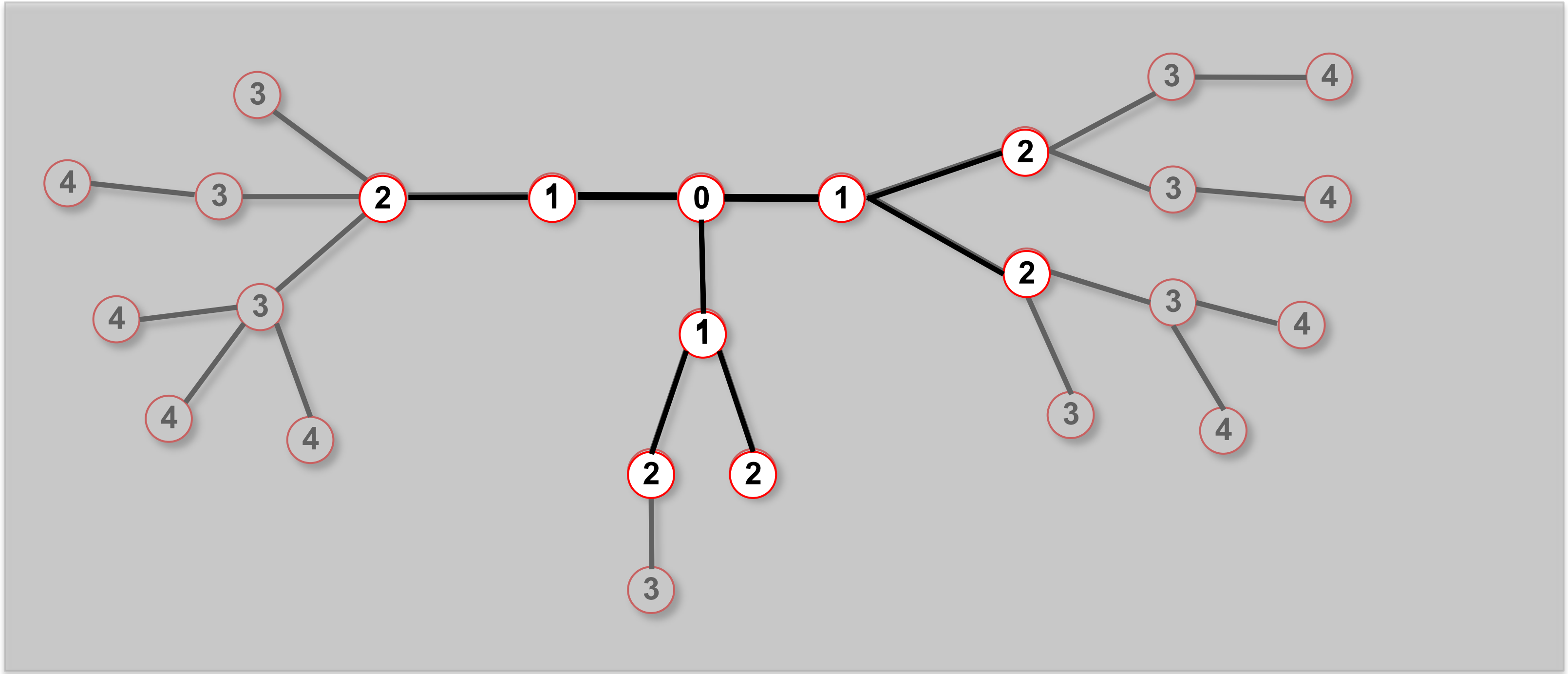
2.Find the nodes adjacent to 1. Mark them as at distance 1. Put them in a queue.



FINDING DISTANCES: BREADTH FIRST SEARCH

Distance between node 0 and node 4:

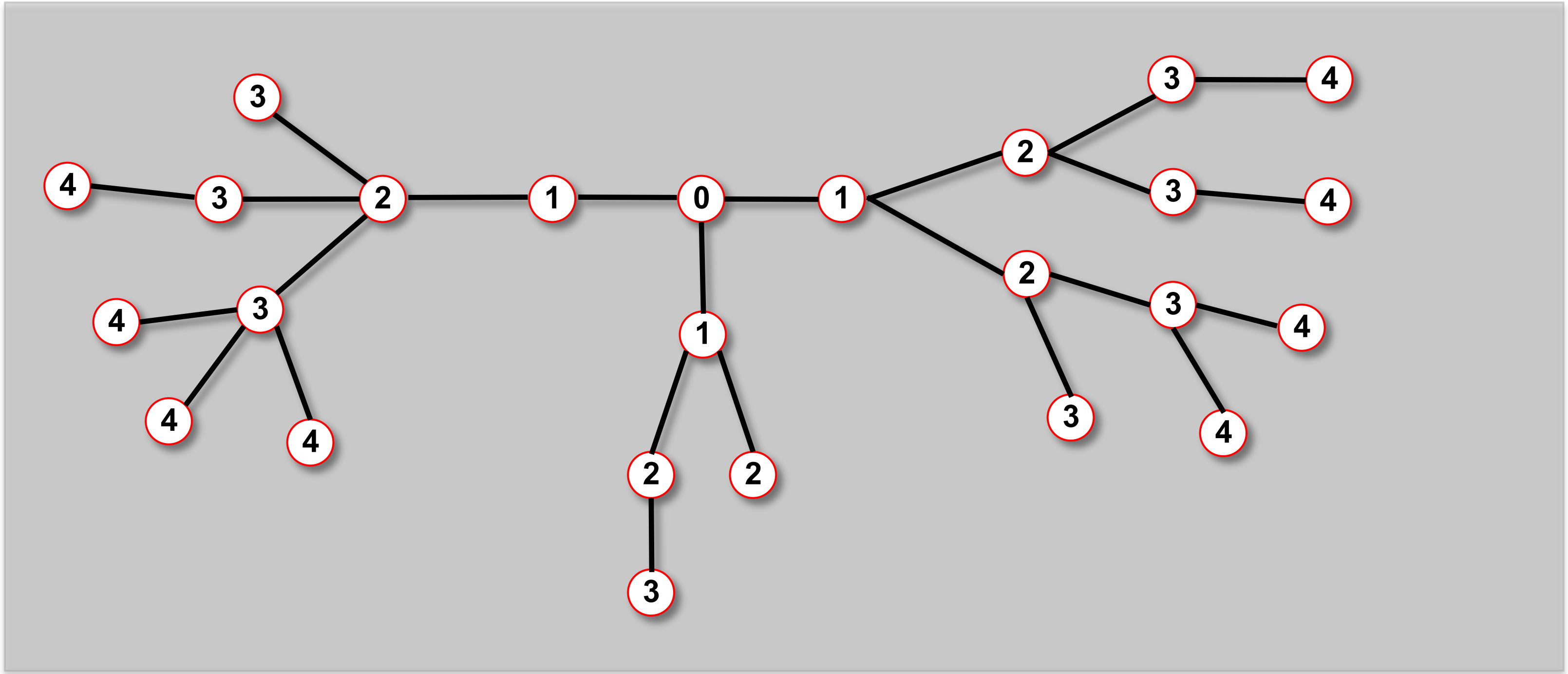
1. Start at 0.
2. Find the nodes adjacent to 0. Mark them as at distance 1. Put them in a queue.
3. Take the first node out of the queue. Find the unmarked nodes adjacent to it in the graph. Mark them with the label of 2. Put them in the queue.



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:

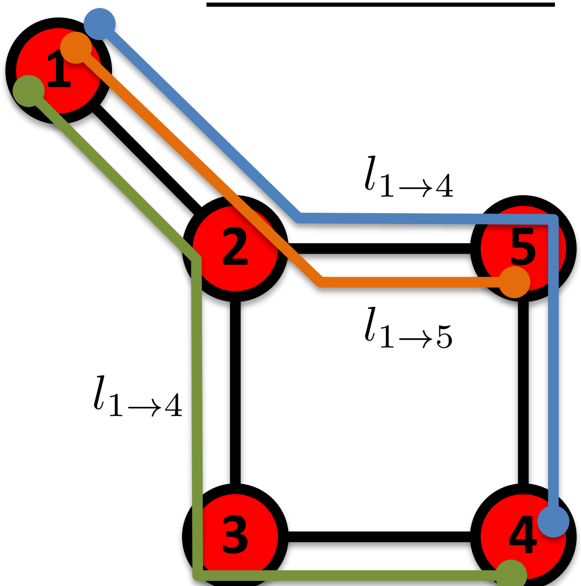
where d_{ij} is the distance from node *i* to node j

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

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

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

Shortest Path



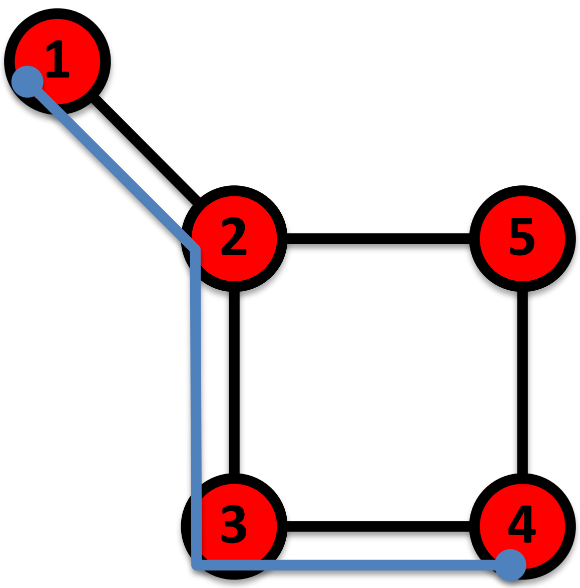
$$l_{1\to4} = 3$$

$$l_{1\to5} = 2$$

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

PATHOLOGY: summary

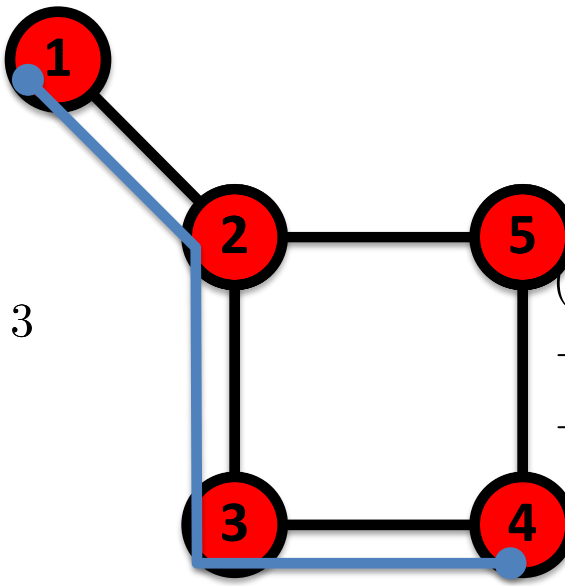
Diameter



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

The longest shortest path in a graph

Average Path Length

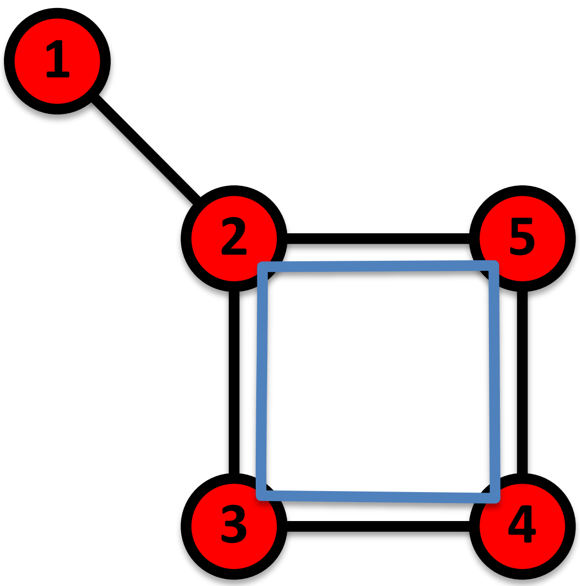


$$(l_{1\to 2} + l_{1\to 3} + l_{1\to 4} + l_{1\to 5} + l_{2\to 3} + l_{2\to 4} + l_{2\to 5} + l_{3\to 4} + l_{3\to 5} + l_{4\to 5})/10 = 1.6$$

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

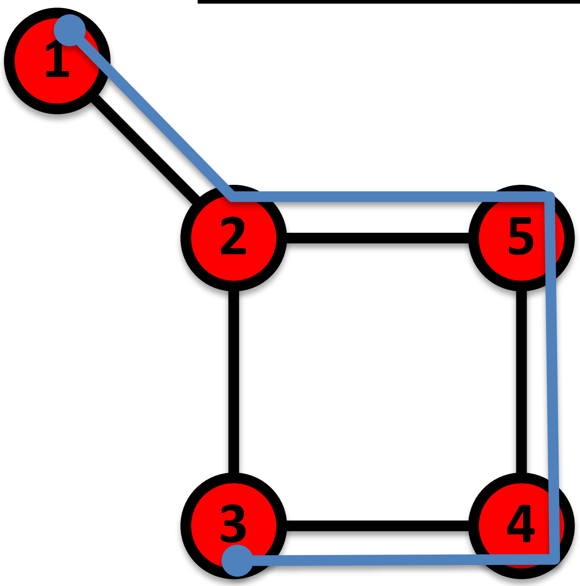
PATHOLOGY: summary

<u>Cycle</u>



A path with the same start and end node.

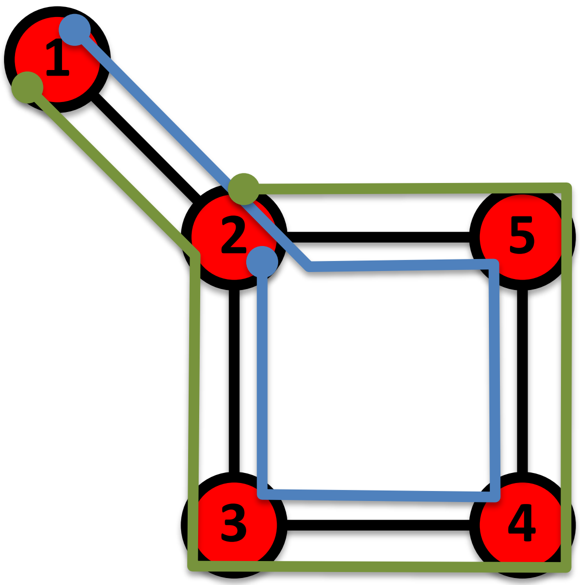
<u>Self-avoiding Path</u>



A path that does not intersect itself.

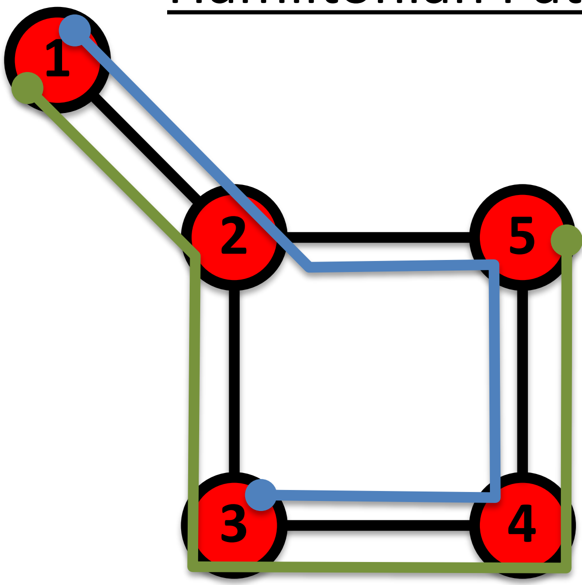
PATHOLOGY: summary

Eulerian Path



A path that traverses each link exactly once.

Hamiltonian Path



A path that visits each node exactly once.