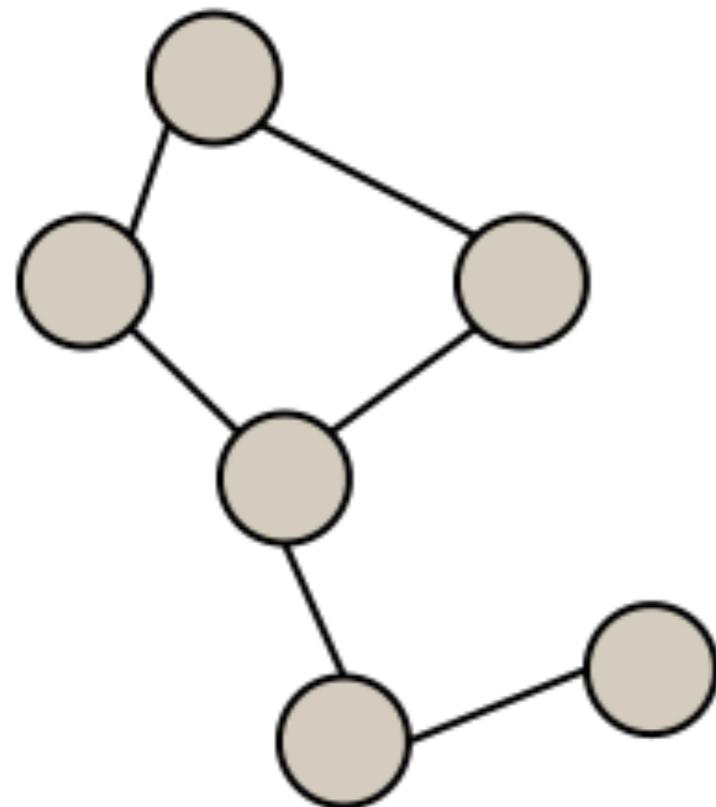


Basic graph theory

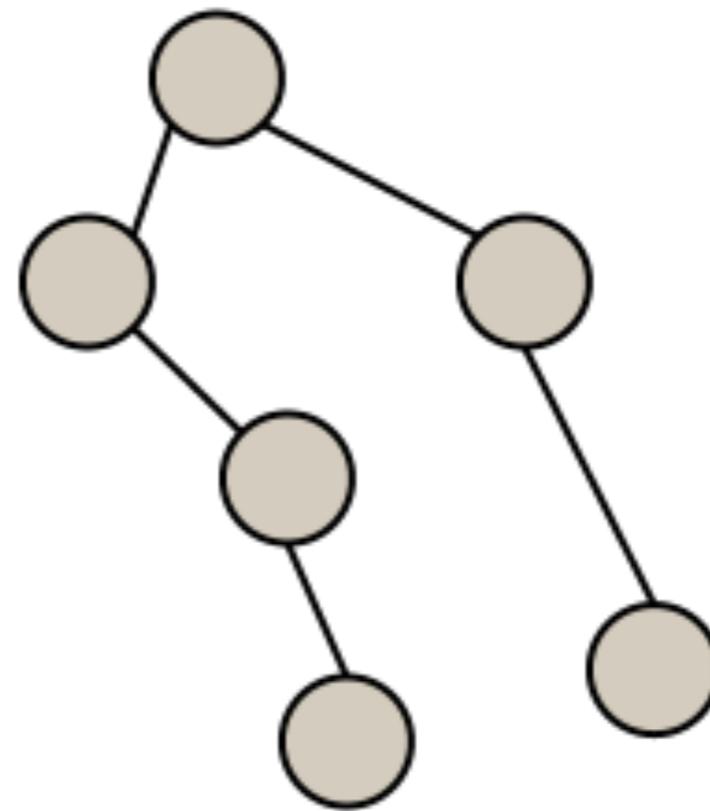
18.S995 - L30-31

dunkel@math.mit.edu

Graphs & Trees



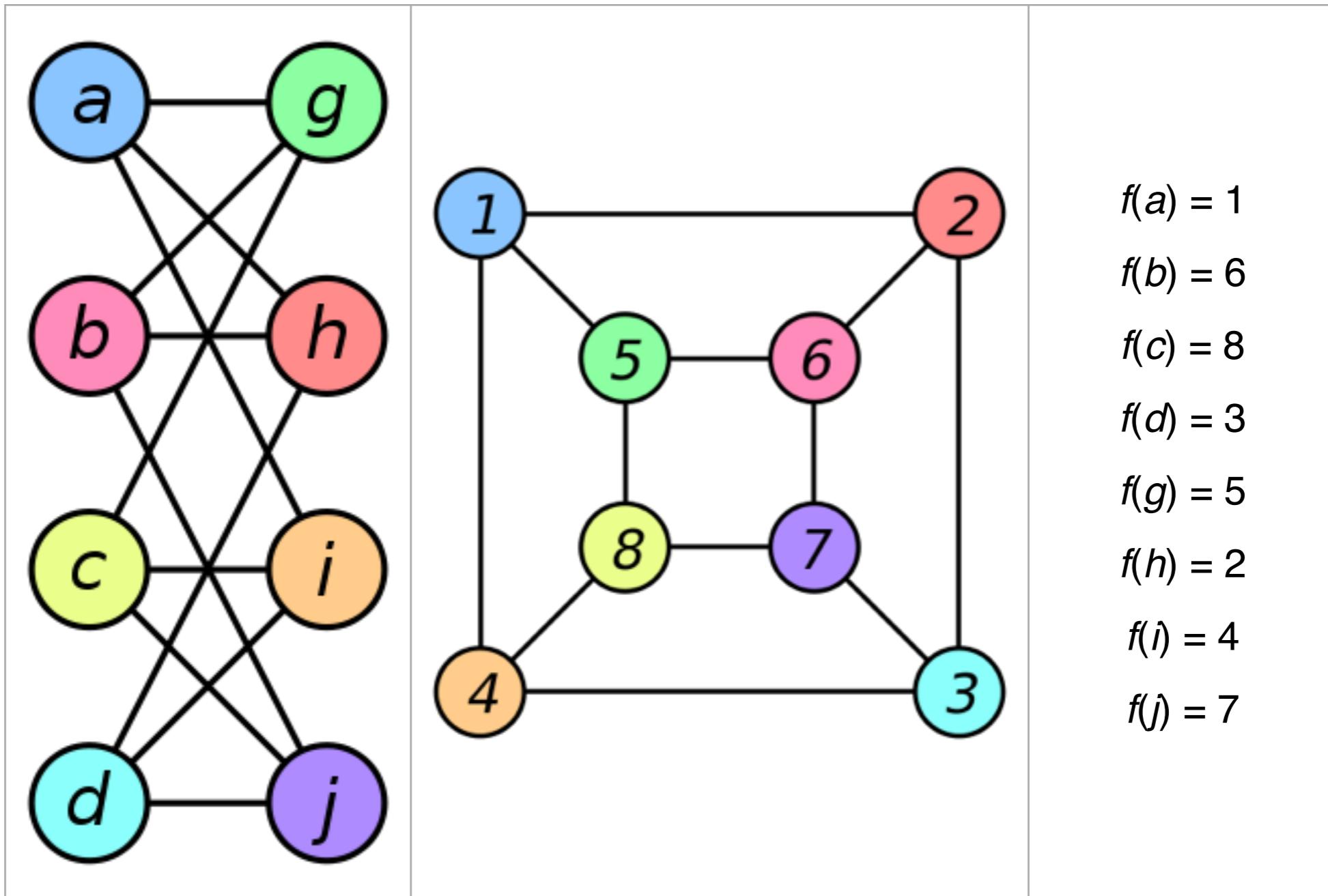
Graph



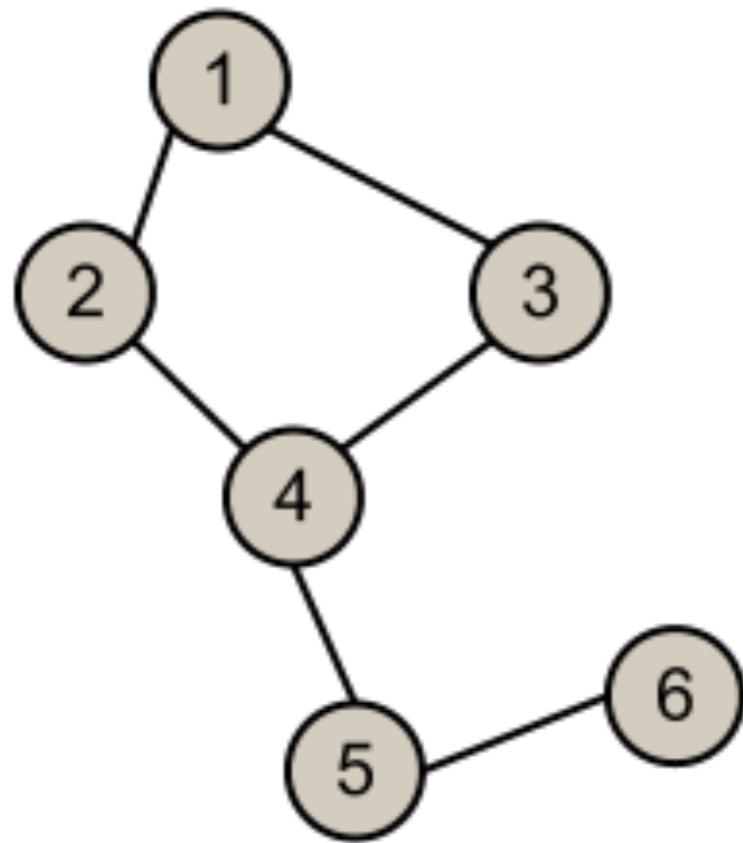
Tree

no cycles

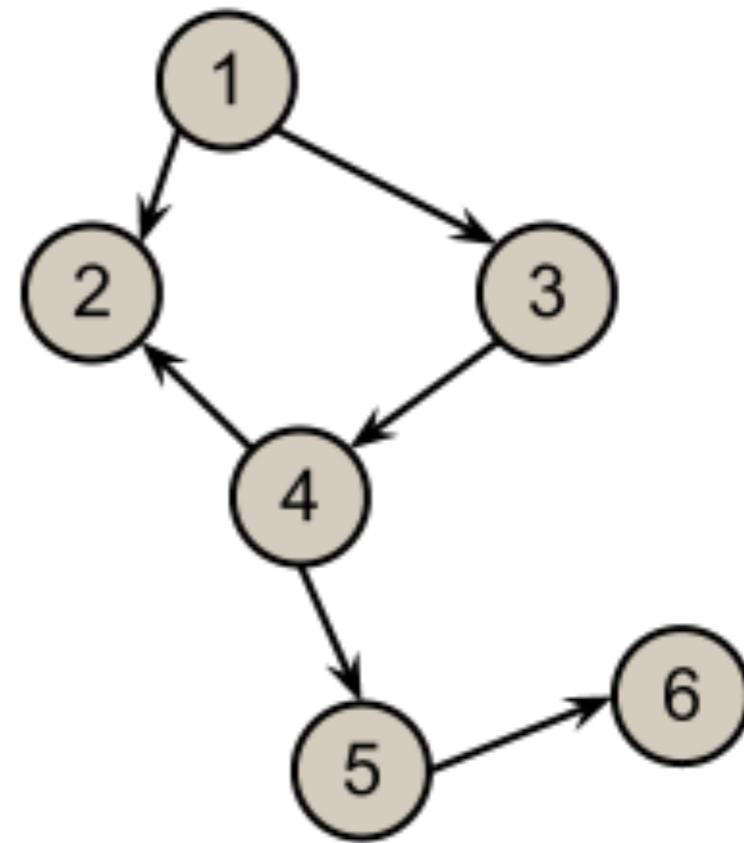
Isomorphic graphs



Directed Graph

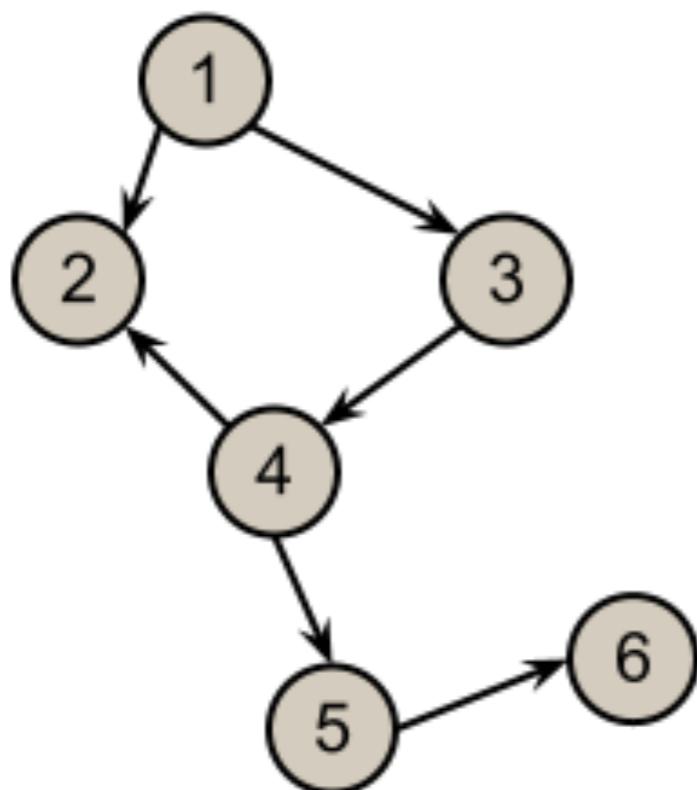


Undirected

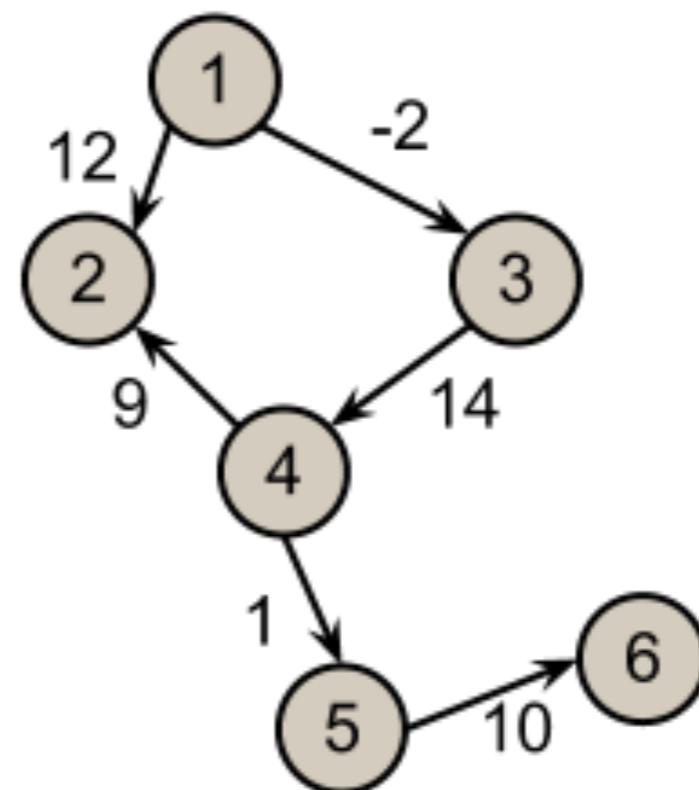


Directed

Weighted Graph

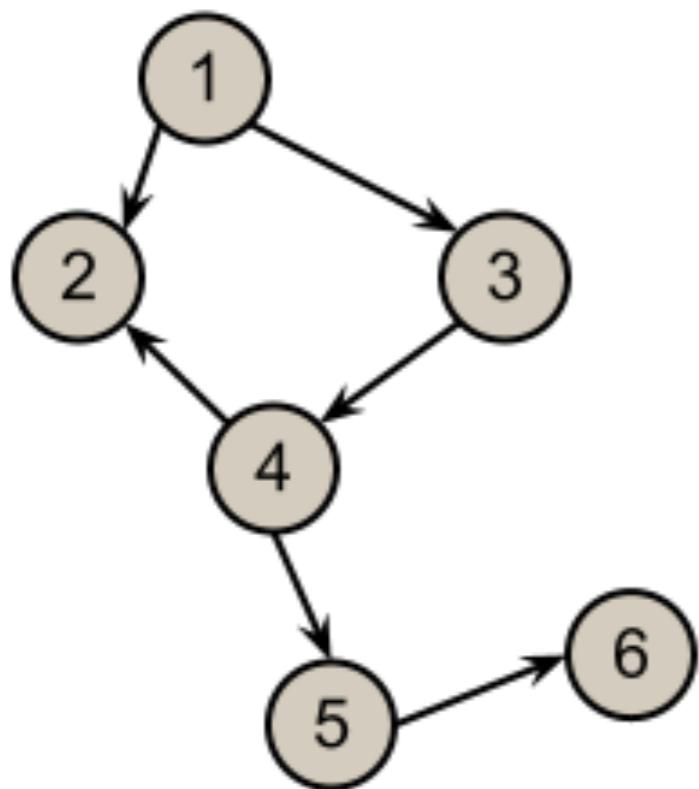


Unweighted

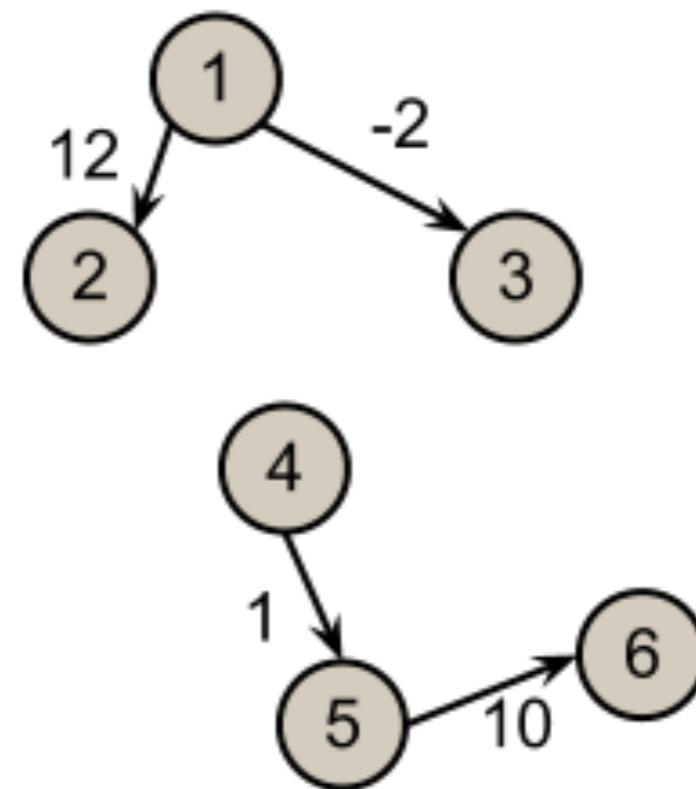


Weighted

Connected Graph

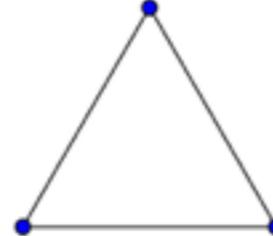
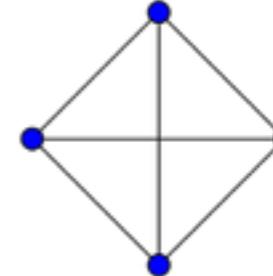
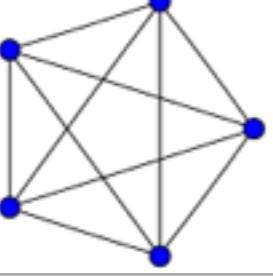
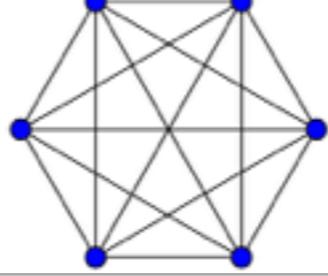
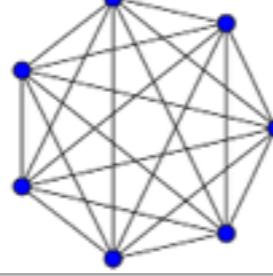
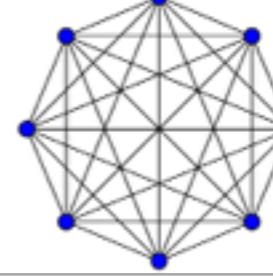
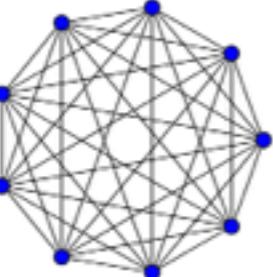
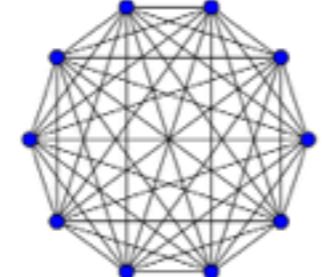
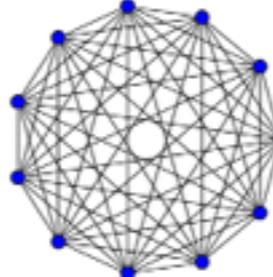
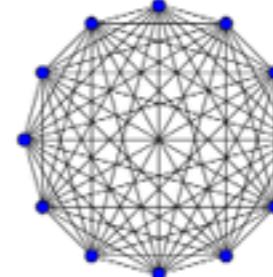


Connected

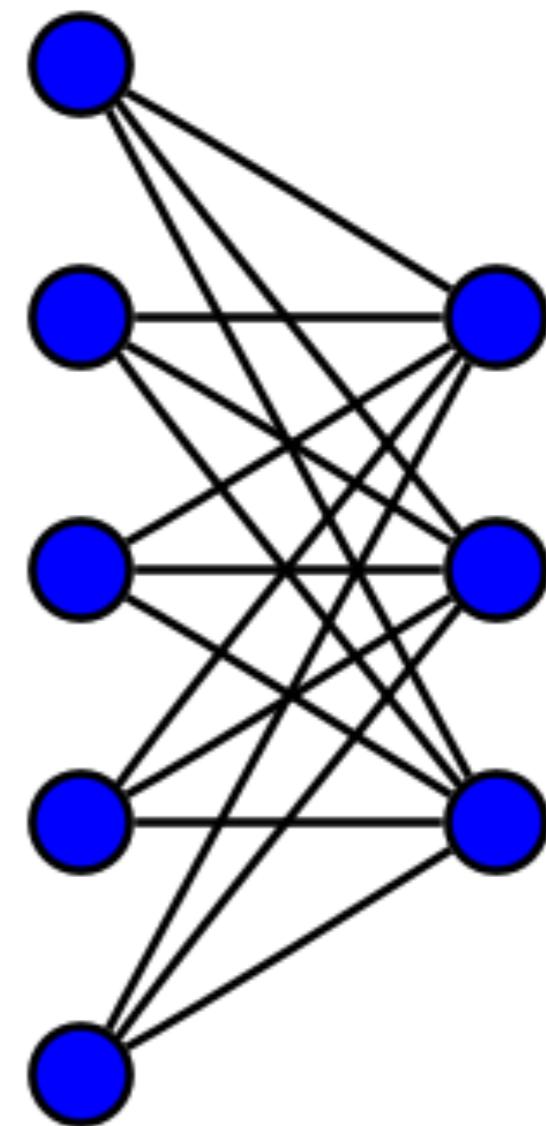
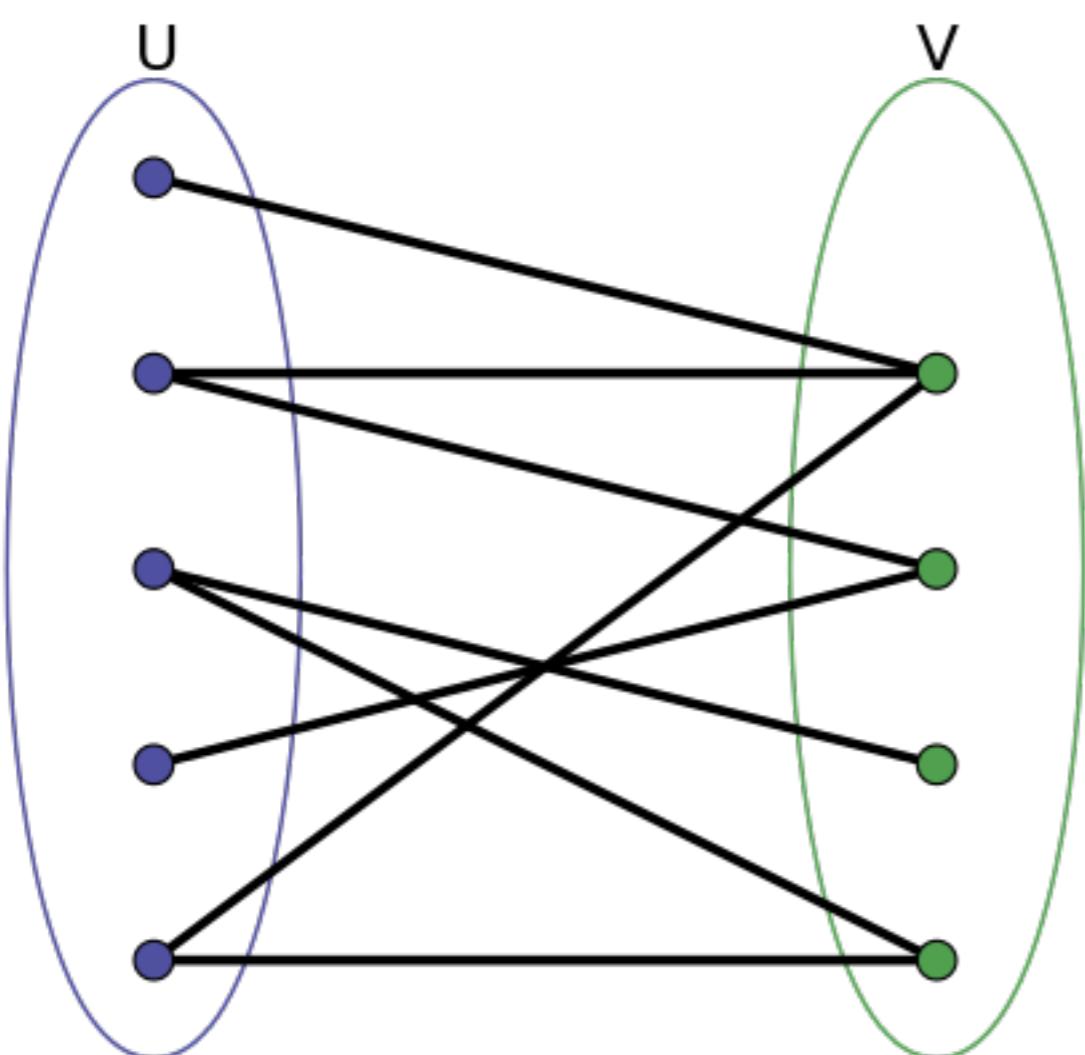


Disconnected

Complete simple graphs on n vertices

K_1	K_2	K_3	K_4
			
K_5	K_6	K_7	K_8
			
K_9	K_{10}	K_{11}	K_{12}
			

Bi-partite graph



Planar, non-planar & dual graphs

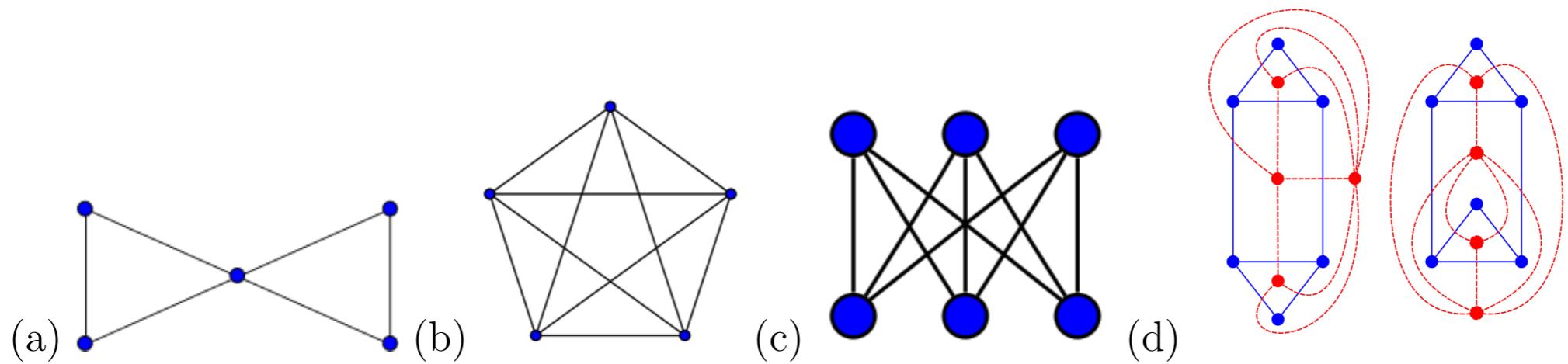
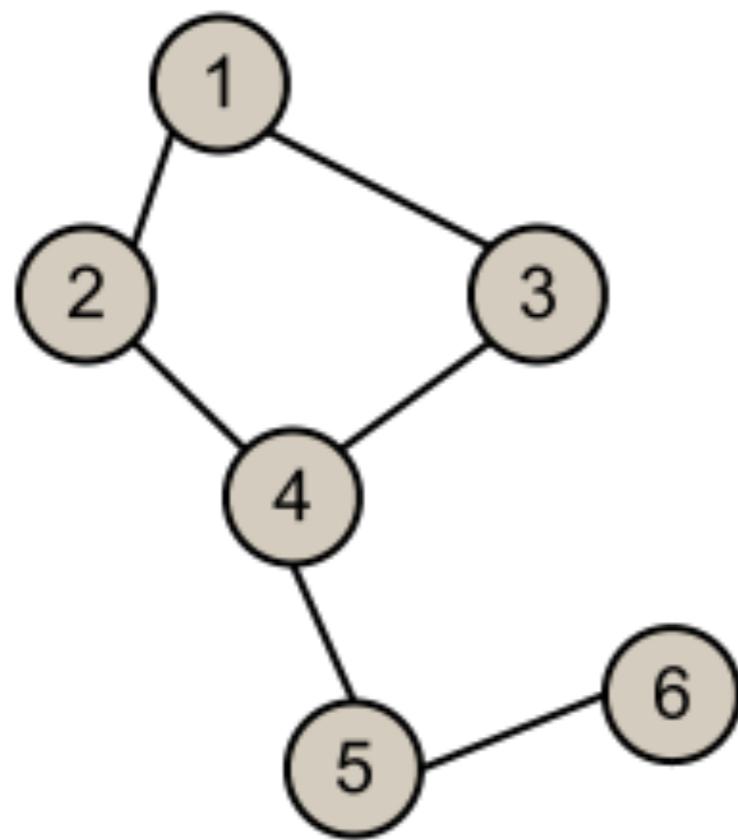


Figure 1.2: Planar, non-planar and dual graphs. (a) Plane ‘butterfly’graph. (b, c) Non-planar graphs. (d) The two red graphs are both dual to the blue graph but they are not isomorphic. Image source: wiki.

Algebraic characterization

Undirected Graph & Adjacency Matrix



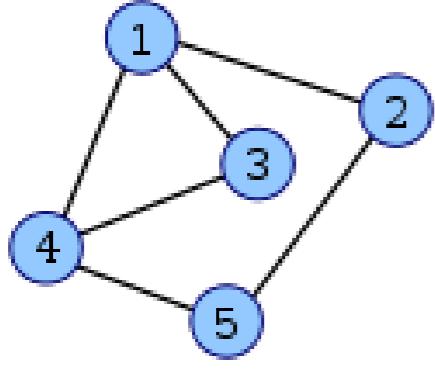
Undirected Graph

	1	2	3	4	5	6
1	0	1	1	0	0	0
2	1	0	0	1	0	0
3	1	0	0	1	0	0
4	0	1	1	0	1	0
5	0	0	0	1	0	1
6	0	0	0	0	1	0

Adjacency Matrix

$|V| \times |V|$ matrix

Characteristic polynomial



$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \end{pmatrix} \quad (1.1)$$

If the graph is simple, then the diagonal elements of \mathbf{A} are zero.

The *characteristic polynomial of a graph* is defined as the characteristic polynomial of the adjacency matrix

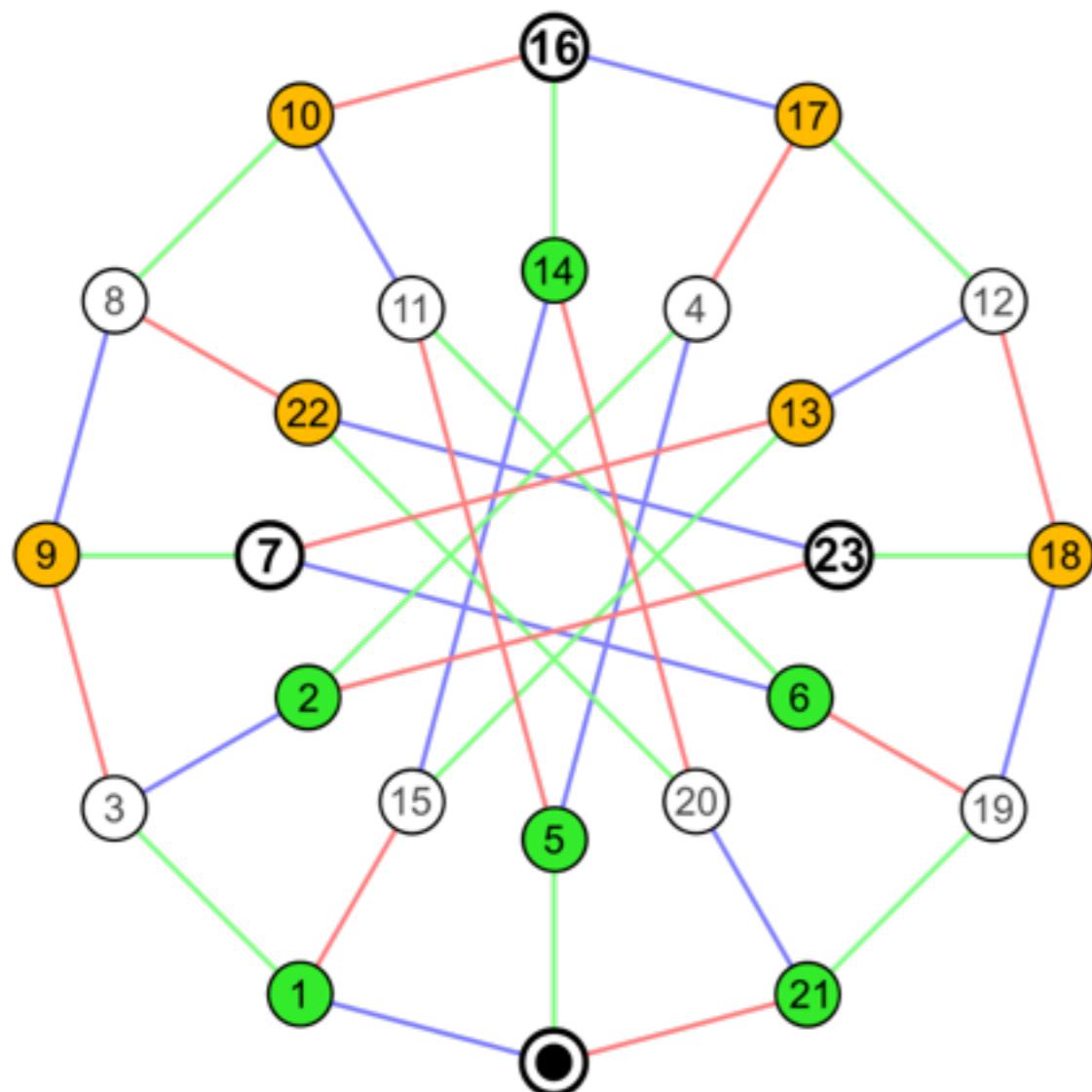
$$p(\mathcal{G}; x) = \det(\mathbf{A} - x\mathbf{I}) \quad (1.7)$$

For the graph in Fig. 1.3a, we find

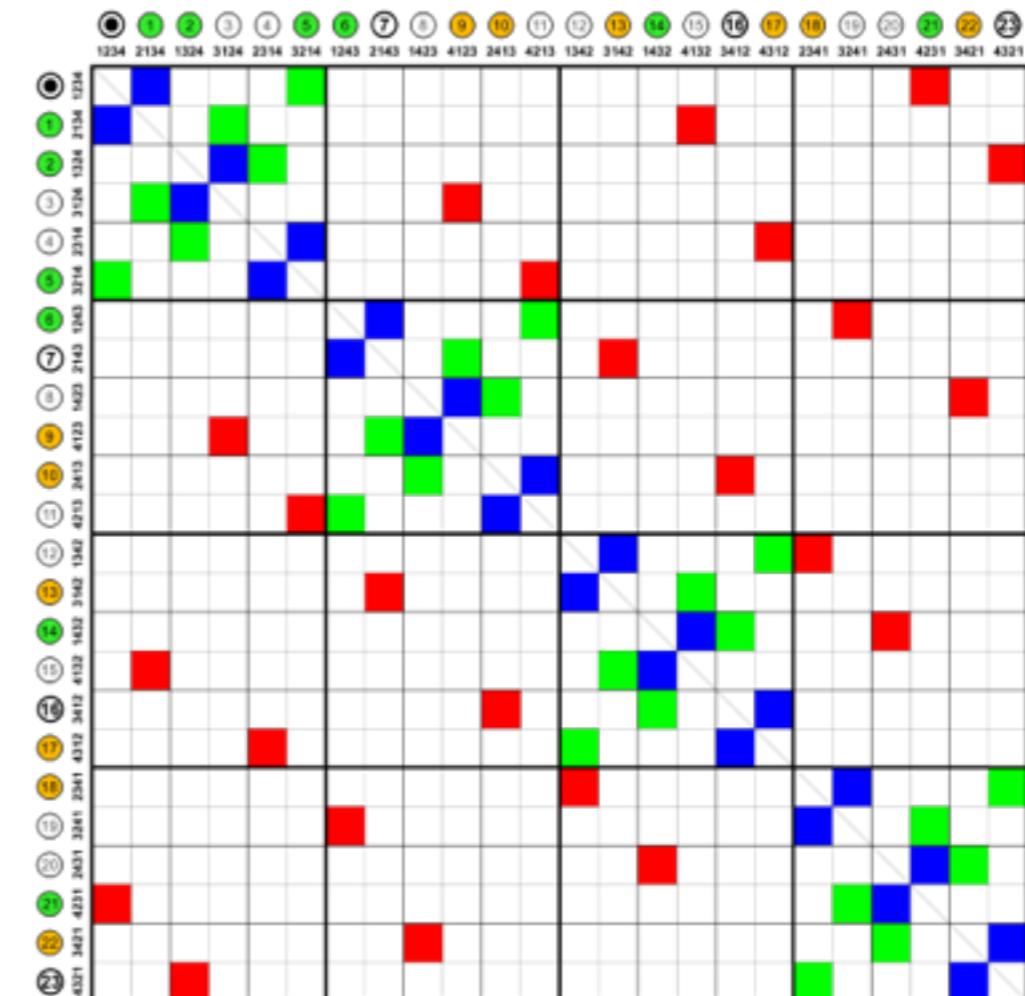
$$p(\mathcal{G}; x) = -x(4 - 2x - 6x^2 + x^4) \quad (1.8)$$

Characteristic polynomials are *not* diagnostic for graph isomorphism, i.e., two nonisomorphic graphs may share the same characteristic polynomial.

Adjacency matrix



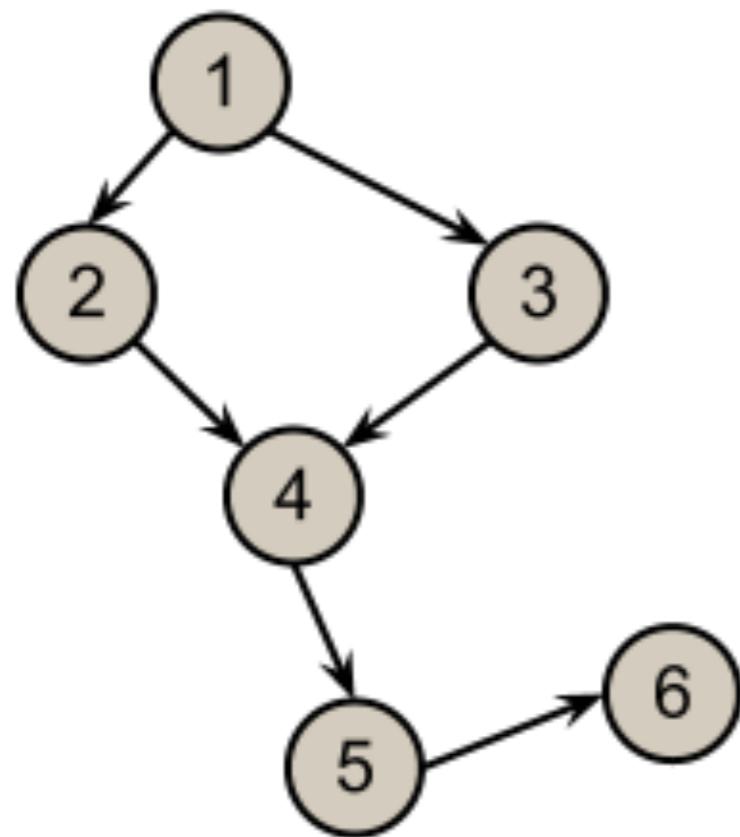
Nauru graph



“integer graph”

$$(x-3)(x-2)^6(x-1)^3x^4(x+1)^3(x+2)^6(x+3),$$

Directed Graph & Adjacency Matrix



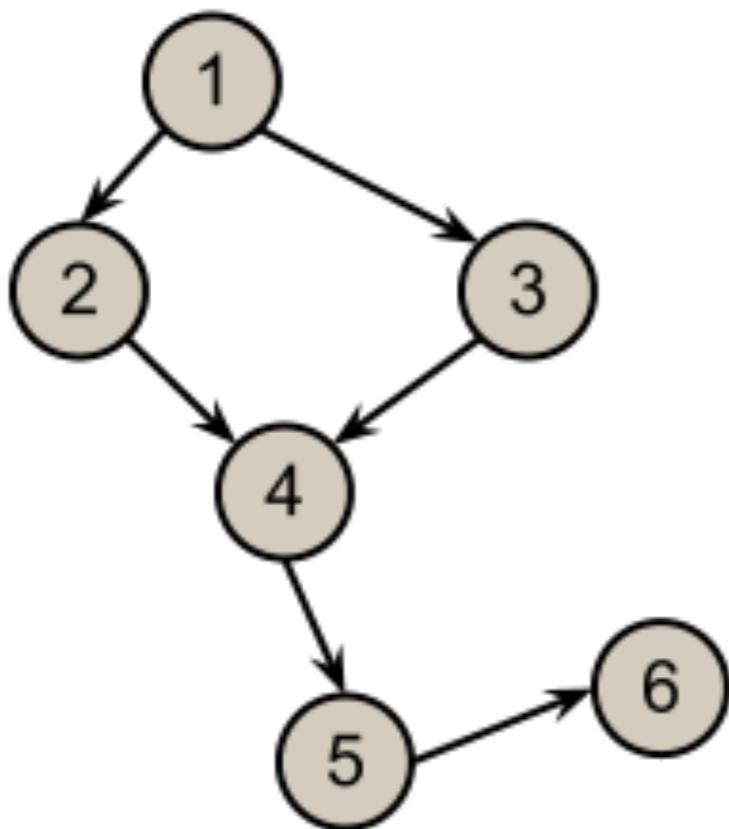
Undirected Graph

	1	2	3	4	5	6
1	0	1	1	0	0	0
2	-1	0	0	1	0	0
3	-1	0	0	1	0	0
4	0	-1	-1	0	1	0
5	0	0	0	-1	0	1
6	0	0	0	0	-1	0

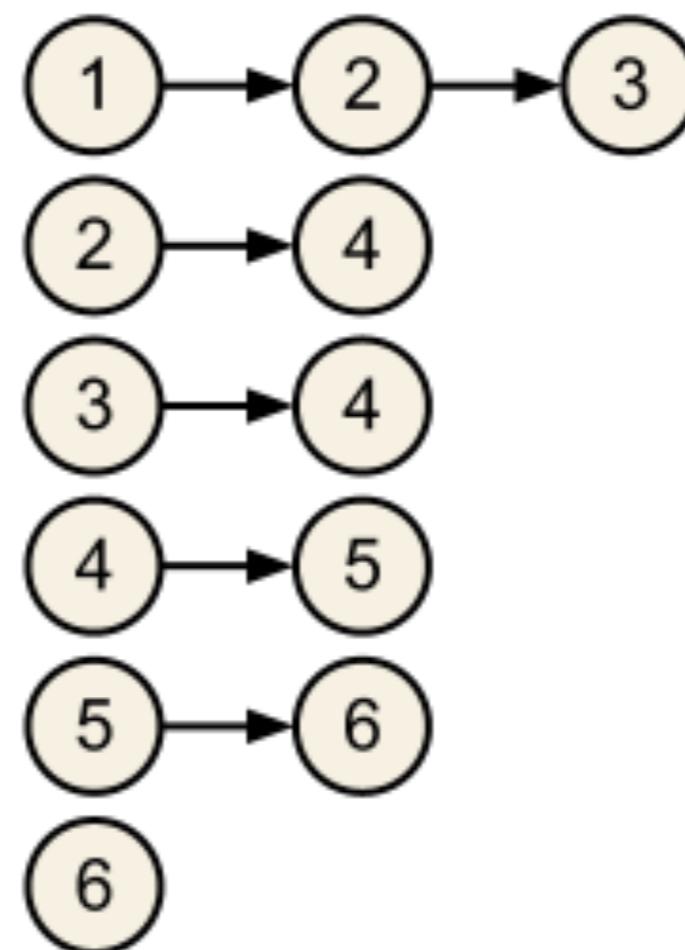
Adjacency Matrix

$|V| \times |V|$ matrix

Directed Graph & Adjacency List



Undirected Graph

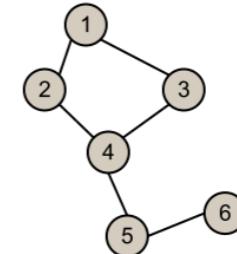


Adjacency List

Complexity

Basic operations in a graph are:

1. Adding an edge
2. Deleting an edge
3. Answering the question “is there an edge between i and j ”
4. Finding the successors of a given vertex
5. Finding (if exists) a path between two vertices



Undirected Graph

	1	2	3	4	5	6
1	0	1	1	0	0	0
2	1	0	0	1	0	0
3	1	0	0	1	0	0
4	0	1	1	0	1	0
5	0	0	0	1	0	1
6	0	0	0	0	1	0

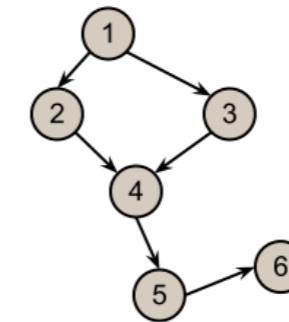
Adjacency Matrix

Complexity

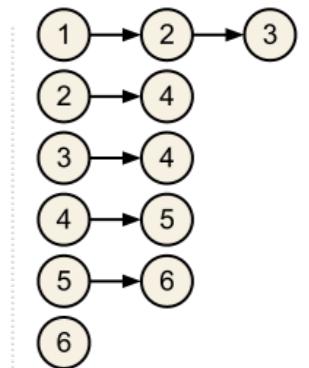
In case that we're using **adjacency matrix** we have:

1. Adding an edge – $O(1)$
2. Deleting an edge – $O(1)$
3. Answering the question “is there an edge between i and j ” – $O(1)$
4. Finding the successors of a given vertex – $O(n)$
5. Finding (if exists) a path between two vertices – $O(n^2)$

Complexity



Undirected Graph

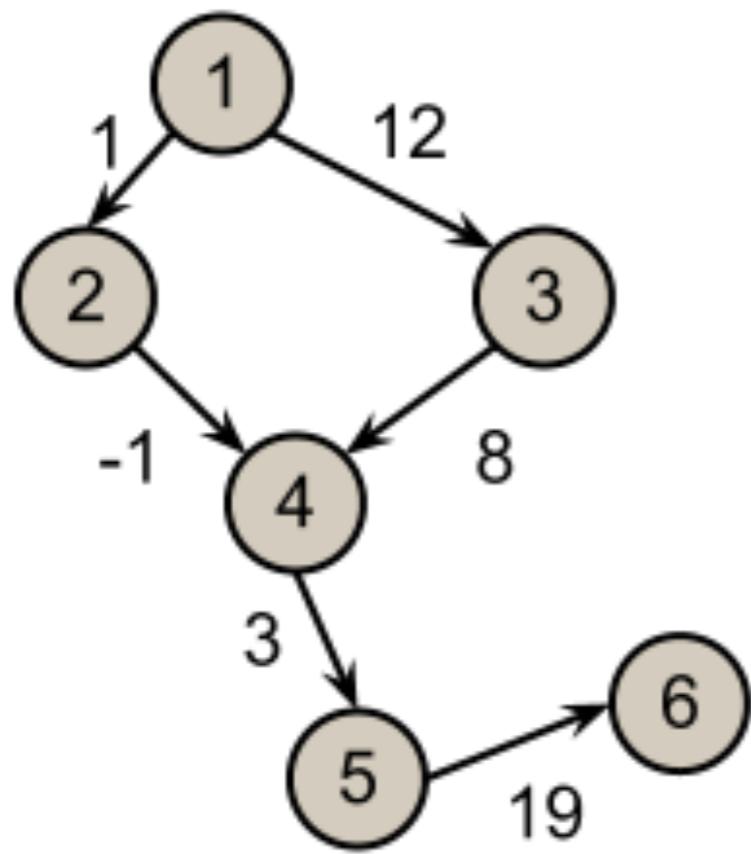


Adjacency List

While for an **adjacency list** we can have:

1. Adding an edge – $O(\log(n))$
2. Deleting an edge – $O(\log(n))$
3. Answering the question “is there an edge between i and j ” – $O(\log(n))$
4. Finding the successors of a given vertex – $O(k)$, where “ k ” is the length of the lists containing the successors of i
5. Finding (if exists) a path between two vertices – $O(n+m)$ with $m \leq n$

Weighted Directed Graph & Adjacency Matrix

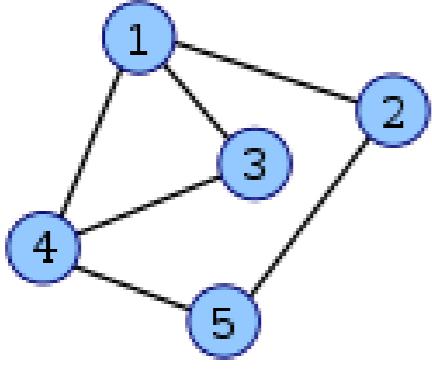


Weighted Directed Graph

1	2	3	4	5	6
1	0	1	12	0	0
2	-1	0	0	-1	0
3	-12	0	0	8	0
4	0	1	-8	0	3
5	0	0	0	-3	0
6	0	0	0	0	-19

Adjacency Matrix

Degree matrix



$$A = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \end{pmatrix} \quad (1.1)$$

If the graph is simple, then the diagonal elements of A are zero.

The column (row) sum defines the *degree* (connectivity) of the vertex

$$\deg(v_i) = \sum_j A_{ij} \quad (1.2)$$

and the volume of the graph is given by

$$\text{vol}(\mathcal{G}) = \sum_V \deg(v_i) = \sum_{ij} A_{ij} \quad (1.3)$$

The degree matrix $D(\mathcal{G})$ is defined as the diagonal matrix

$$D(\mathcal{G}) = \text{diag}(\deg(v_1), \dots, \deg(v_{|V|})) \quad (1.4)$$

For the graph in Fig. 1.3a, one has

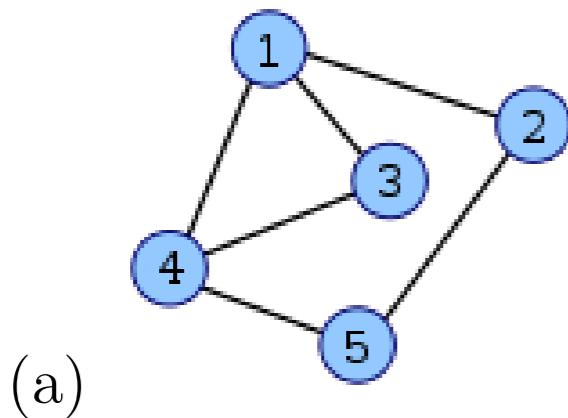
$$D = \begin{pmatrix} 3 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{pmatrix} \quad (1.5)$$

Directed incidence matrix In addition to the undirected incidence matrix \mathbf{C} , we still define a directed $|V| \times |E|$ -matrix $\vec{\mathbf{C}}$ as follows

$$\vec{C}_{is} = \begin{cases} -1, & \text{if edge } e_s \text{ departs from } v_i \\ +1, & \text{if edge } e_s \text{ arrives at } v_i \\ 0, & \text{otherwise} \end{cases} \quad (1.13)$$

For undirected graphs, the assignment of the edge direction is arbitrary – we merely have to ensure that the columns $s = 1, \dots, |E|$ of $\vec{\mathbf{C}}$ sum to 0. For the graph in Fig. 1.3a, one finds

$$\vec{\mathbf{C}} = \begin{pmatrix} -1 & -1 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 1 & -1 \\ 0 & 0 & 0 & 1 & 0 & 1 \end{pmatrix} \quad (1.14)$$



1.3.1 Laplacian

The $|V| \times |V|$ -Laplacian matrix $\mathbf{L}(\mathcal{G})$ of a graph \mathcal{G} , often also referred to as Kirchhoff matrix, is defined as the difference between degree matrix and adjacency matrix

$$\mathbf{L} = \mathbf{D} - \mathbf{A} \quad (1.15a)$$

Hence

$$L_{ij} = \begin{cases} \deg(v_i), & \text{if } i = j \\ -1, & \text{if } v_i \text{ and } v_j \text{ are connected by edge} \\ 0, & \text{otherwise} \end{cases} \quad (1.15b)$$

As we shall see below, this matrix provides an important characterization of the underlying graph.

The $|V| \times |V|$ -Laplacian matrix can also be expressed in terms of the *directed* incidence matrix $\vec{\mathbf{C}}$, as

$$\mathbf{L} = \vec{\mathbf{C}} \cdot \vec{\mathbf{C}}^\top \quad \Leftrightarrow \quad L_{ij} = \vec{C}_{ir} \vec{C}_{jr} \quad (1.16)$$

(a)

$\vec{\mathbf{C}} = \begin{pmatrix} -1 & -1 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 1 & -1 \\ 0 & 0 & 0 & 1 & 0 & 1 \end{pmatrix}$

$\mathbf{L} = \begin{pmatrix} 3 & -1 & -1 & -1 & 0 \\ -1 & 2 & 0 & 0 & -1 \\ -1 & 0 & 2 & -1 & 0 \\ -1 & 0 & -1 & 3 & -1 \\ 0 & -1 & 0 & -1 & 2 \end{pmatrix}$

Normalized Laplacian The associated normalized Laplacian $\bar{\mathbf{L}}(\mathcal{G})$ is defined as

$$\bar{\mathbf{L}} = \mathbf{D}^{-1/2} \cdot \mathbf{L} \cdot \mathbf{D}^{-1/2} = \mathbf{I} - \mathbf{D}^{-1/2} \cdot \mathbf{A} \cdot \mathbf{D}^{-1/2} \quad (1.19a)$$

with elements

$$\bar{L}_{ij} = \begin{cases} 1, & \text{if } i = j \text{ and } \deg(v_i) \neq 0 \\ -1/\sqrt{\deg(v_i) \deg(v_j)}, & \text{if } i \neq j \text{ and } v_i \text{ and } v_j \text{ are connected by edge} \\ 0, & \text{otherwise} \end{cases} \quad (1.19b)$$

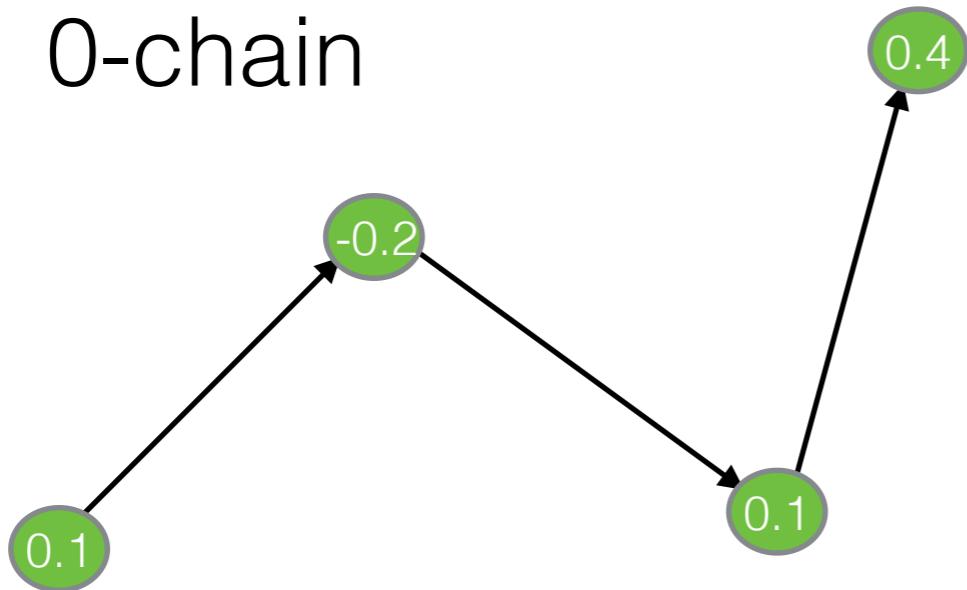
One can write $\bar{\mathbf{L}}(\mathcal{G})$ as, cf. Eq. (1.16),

$$\bar{\mathbf{L}}(\mathcal{G}) = \vec{\mathbf{B}} \cdot \vec{\mathbf{B}}^\top \quad (1.20a)$$

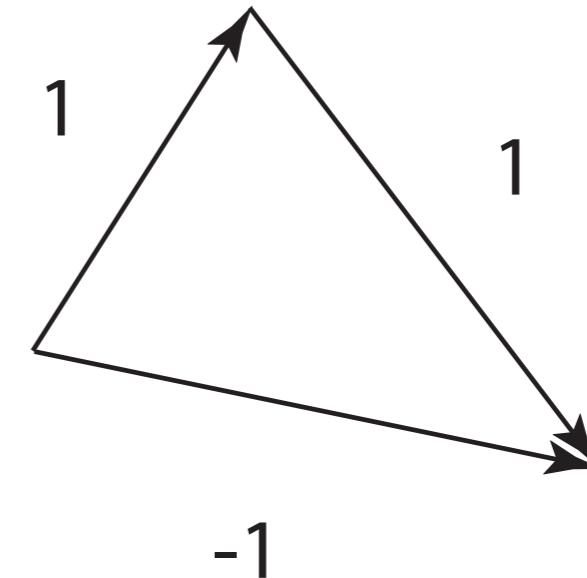
where $\vec{\mathbf{B}}$ is an $|V| \times |E|$ -matrix where

$$\vec{B}_{is} = \begin{cases} -1/\sqrt{\deg(v_i)}, & \text{if edge } e_s \text{ departs from } v_i \\ +1/\sqrt{\deg(v_i)}, & \text{if edge } e_s \text{ arrives at } v_i \\ 0, & \text{otherwise} \end{cases} \quad (1.20b)$$

0-chain



1-chain



A ‘0-chain’ is a real-valued vertex function $g : V \rightarrow \mathbb{R}$, and a ‘1-chain’ is a real-valued edge function $E \rightarrow \mathbb{R}$. Then $\vec{B} = (\vec{B}_{is})$ can be viewed as *boundary operator* that maps 1-chains onto 0-chains, while the transposed matrix $\vec{B}^\top = (\vec{B}_{si})$ is a *co-boundary operator* that maps 0-chains onto 1-chains. Accordingly \vec{L} can be viewed as an operator that maps vertex functions \mathbf{g} , which can be viewed as $|V|$ -dimensional column vector, onto another vertex function $\vec{L} \cdot \mathbf{g}$, such that

$$(\vec{L} \cdot \mathbf{g})(v_i) = \frac{1}{\sqrt{\deg(v_i)}} \sum_{v_j \sim v_i} \left[\frac{g(v_i)}{\sqrt{\deg(v_i)}} - \frac{g(v_j)}{\sqrt{\deg(v_j)}} \right] \quad (1.21)$$

where $v_j \sim v_i$ denotes the set of adjacent nodes.

We denote the eigenvalues of $\bar{\mathbf{L}}$ by

$$0 = \bar{\lambda}_0 \leq \bar{\lambda}_1 \leq \dots \leq \bar{\lambda}_{|V|-1} \quad (6.22)$$

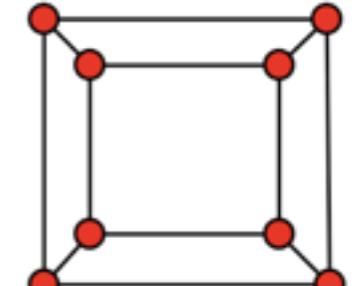
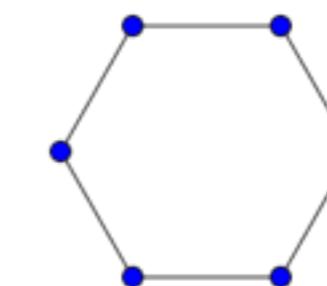
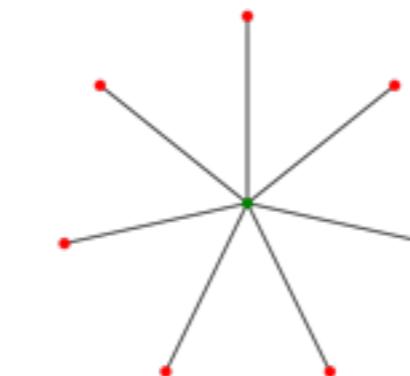
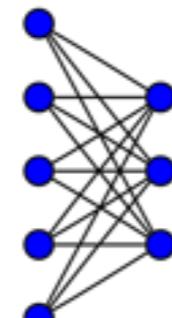
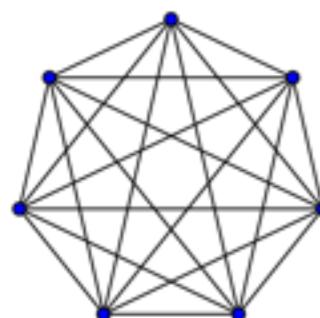
Abbreviating $n = |V|$, one can show that

- (i) $\sum_i \bar{\lambda}_i \leq n$ with equality iff \mathcal{G} has no isolated vertices.
- (ii) $\bar{\lambda}_1 \leq n/(n-1)$ with equality iff \mathcal{G} is the complete graph on $n \geq 2$ vertices.
- (iii) If $n \geq 2$ and \mathcal{G} has no isolated vertices, then $\bar{\lambda}_{n-1} \geq n/(n-1)$.
- (iv) If \mathcal{G} is not complete, then $\bar{\lambda}_1 \leq 1$.
- (v) If \mathcal{G} is connected, then $\bar{\lambda}_1 > 0$.
- (vi) If $\bar{\lambda}_i = 0$ and $\bar{\lambda}_{i+1} > 0$, then \mathcal{G} has exactly $i+1$ connected components.
- (vii) For all $i \leq n-1$, we have $\lambda_i \leq 2$, with $\bar{\lambda}_{n-1} = 2$ iff a connected component of \mathcal{G} is bipartite and nontrivial.
- (viii) The spectrum of a graph is the union of the spectra of its connected components.

See Chapter 1 in [Chu97] for proofs.

Examples:

- For a complete graph K_n on $n \geq 2$ vertices, the eigenvalues are 0 (multiplicity 1) and $n/(n - 1)$ (multiplicity $n - 1$)
- For a complete bipartite graph $K_{m,n}$ on $m + n$ vertices, the eigenvalues are 0 and 1 (multiplicity $m + n - 2$) and 2.
- For the star S_n on $n \geq 2$ vertices, the eigenvalues are 0 and 1 (multiplicity $n - 2$) and 2.
- For the path P_n on $n \geq 2$ vertices, the eigenvalues are $\bar{\lambda}_k = 1 - \cos[\pi k/(n - 1)]$ for $k = 0, \dots, n - 1$.
- For the cycle C_n on $n \geq 2$ vertices, the eigenvalues are $\bar{\lambda}_k = 1 - \cos[2\pi k/n]$ for $k = 0, \dots, n - 1$.
- For the n -cube Q_n on 2^n vertices, the eigenvalues are $\bar{\lambda}_k = 2k/n$, with multiplicity $\binom{n}{k}$ for $k = 0, \dots, n$.



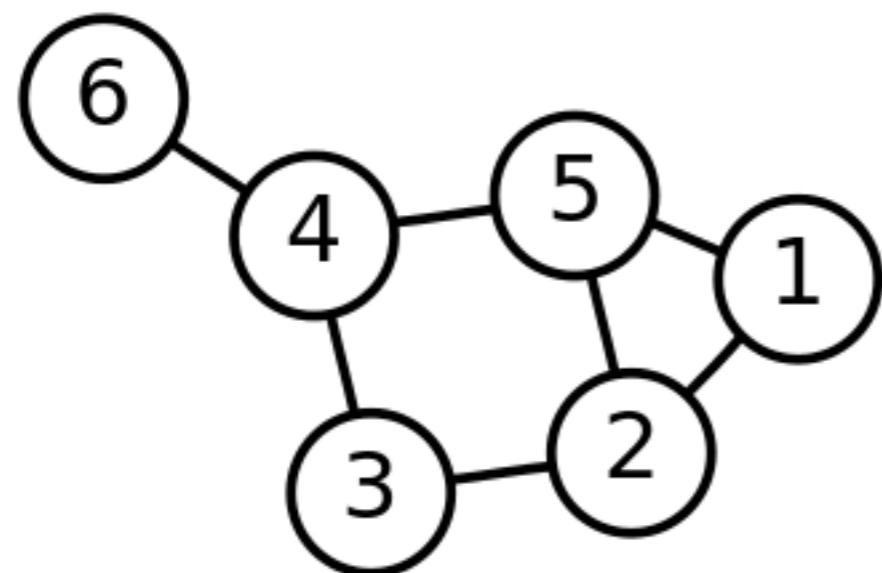
Graph Laplacian

$$L = D - A$$

$$L_{ij} = \begin{cases} \deg(v_i), & \text{if } i = j \\ -1, & \text{if } v_i \text{ and } v_j \text{ are connected by edge} \\ 0, & \text{otherwise} \end{cases}$$

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

degree matrix



$$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

adjacency matrix

$$\begin{pmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & -1 & 0 & -1 & 3 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$$

Laplacian matrix

Properties We denote the eigenvalues of \mathbf{L} by

$$\lambda_0 \leq \lambda_1 \leq \dots \leq \lambda_{|V|} \quad (1.18)$$

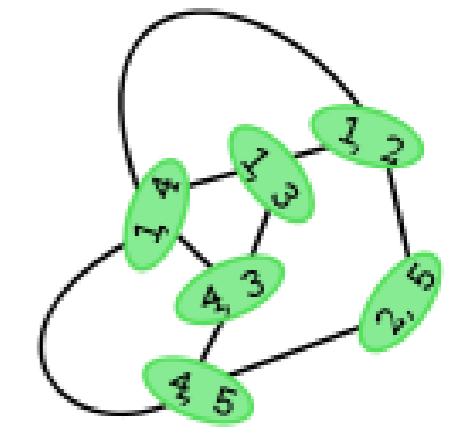
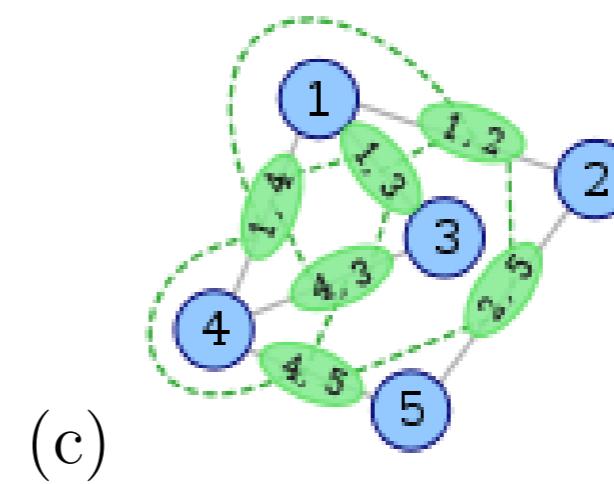
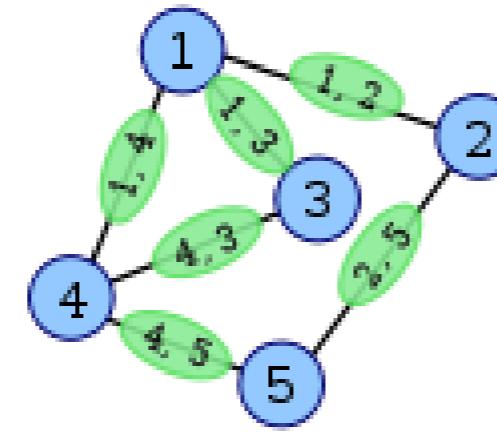
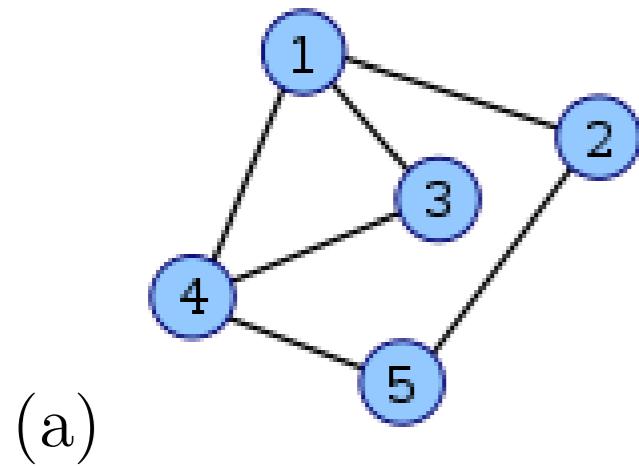
The following properties hold:

- (i) \mathbf{L} is symmetric.
- (ii) \mathbf{L} is positive-semidefinite, that is $\lambda_i \geq 0$ for all i .
- (iii) Every row sum and column sum of \mathbf{L} is zero.²
- (iv) $\lambda_0 = 0$ as the vector $\mathbf{v}_0 = (1, 1, \dots, 1)$ satisfies $\mathbf{L} \cdot \mathbf{v}_0 = \mathbf{0}$.
- (v) The multiplicity of the eigenvalue 0 of the Laplacian equals the number of connected components in the graph.
- (vi) The smallest non-zero eigenvalue of \mathbf{L} is called the spectral gap.
- (vii) For a graph with multiple connected components, \mathbf{L} can be written as a block diagonal matrix, where each block is the respective Laplacian matrix for each component.

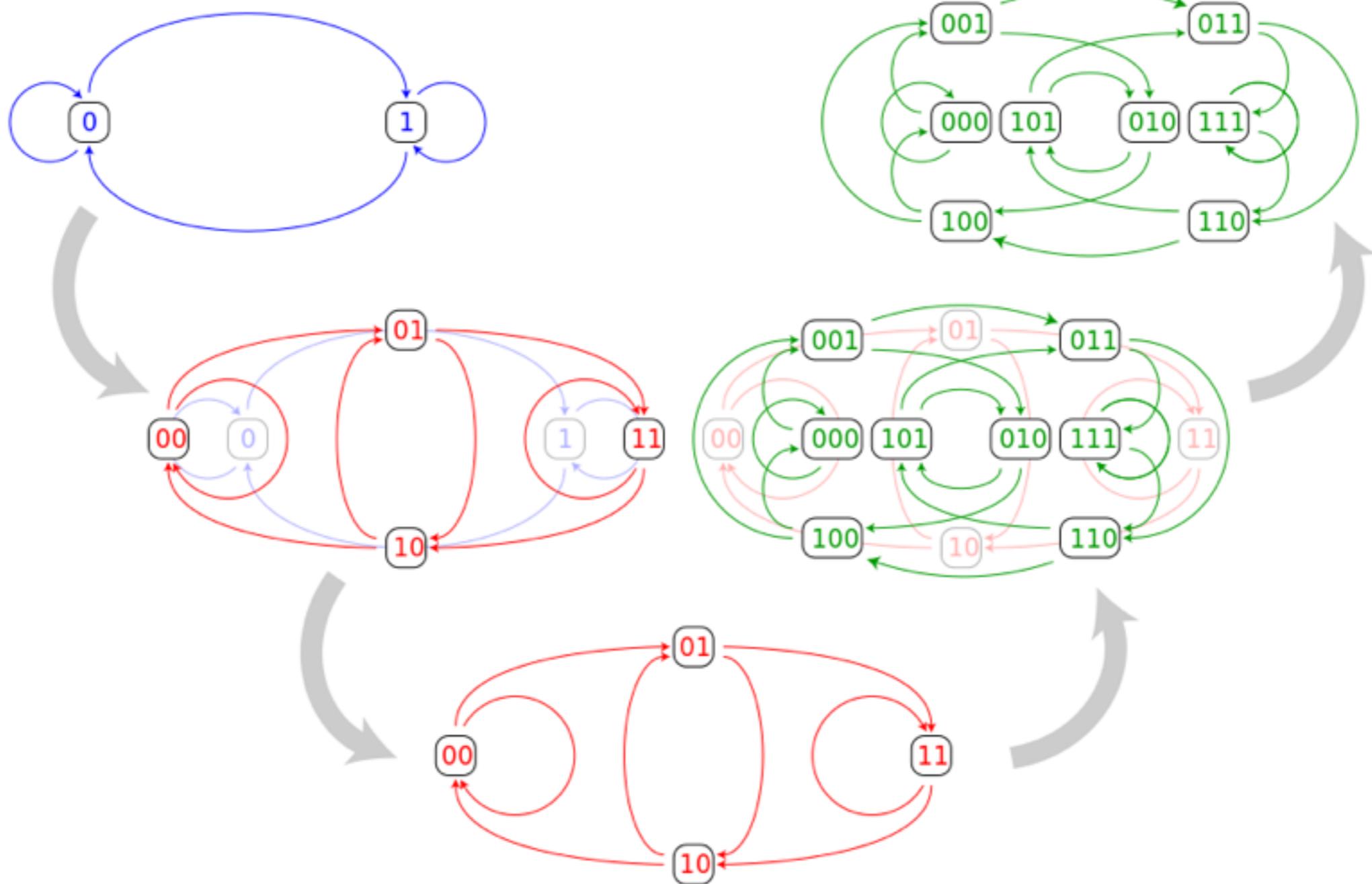
²The degree of the vertex is summed with a -1 for each neighbor

Line graphs of undirected graphs

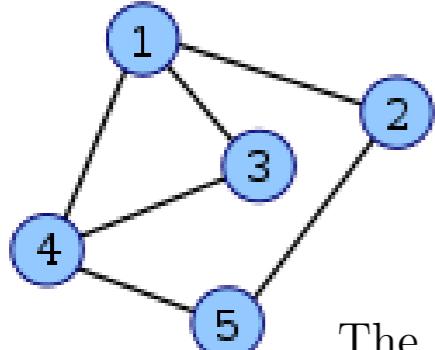
1. draw vertex for each edge in G
2. connect vertices if edges have joint point



Line graphs of directed graphs



Incidence matrix The incidence matrix \mathbf{C} of graph \mathcal{G} is a $|V| \times |E|$ -matrix with $C_{is} = 1$ if edge v_i is contained in edge e_s , and $C_{is} = 0$ otherwise. For the graph in Fig. 1.3a, with $i = 1, \dots, 5$ vertices and $s = 1, \dots, 6$ edges, we have



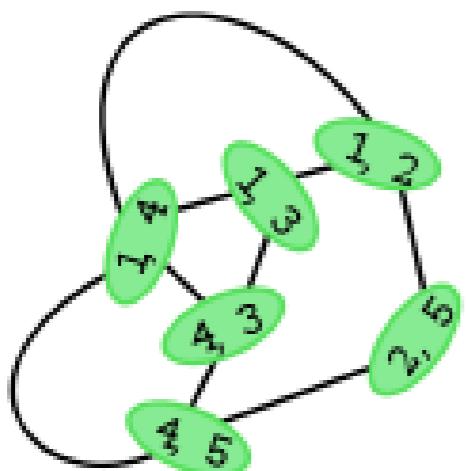
$$\mathbf{C} = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \end{pmatrix} \quad (1.9)$$

The incidence matrix $\mathbf{C}(\mathcal{G})$ of a graph \mathcal{G} and the *adjacency matrix* $A(\mathcal{L}[\mathcal{G}])$ of its line graph $\mathcal{L}[\mathcal{G}]$ are related by

$$\mathbf{A}(\mathcal{L}[\mathcal{G}]) = \mathbf{C}(\mathcal{G})^\top \cdot \mathbf{C}(\mathcal{G}) - 2\mathbf{I} \quad \Leftrightarrow \quad A(\mathcal{L}[\mathcal{G}])_{rs} = C_{ir}C_{is} - 2\delta_{rs} \quad (1.10)$$

For the example in Fig. 1.3, we thus find

$$\mathbf{A}(\mathcal{L}[\mathcal{G}]) = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 1 & 0 \end{pmatrix} \quad (1.11)$$

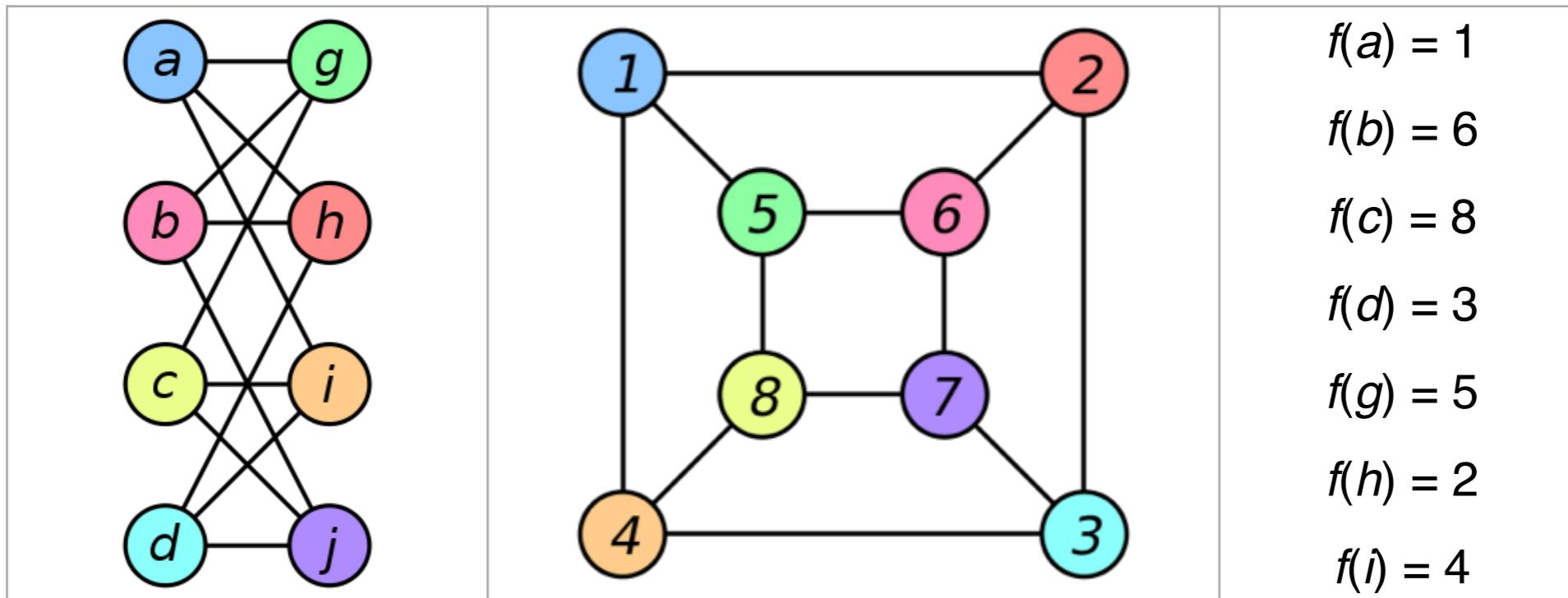


characteristic polynomial

$$p(\mathcal{L}[\mathcal{G}]; x) = (x + 2) (x^2 + x - 1) [(x - 3)x^2 - x + 2]$$

Isomorphic graphs

image source: wiki



Whitney graph isomorphism theorem: Two connected graphs are isomorphic if and only if their [line graphs](#) are isomorphic, with a single exception: K_3 , the [complete graph](#) on three vertices, and the [complete bipartite graph](#) $K_{1,3}$, which are not isomorphic but both have K_3 as their line graph.



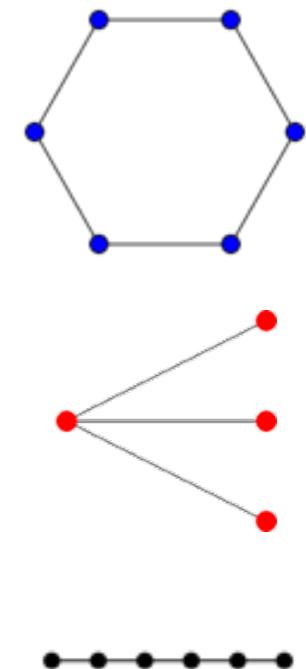
Line graphs of line graphs of

$$G, L(G), L(L(G)), L(L(L(G))), \dots$$

van Rooij & Wilf (1965):

When G is a finite **connected graph**, only four possible behaviors are possible for this sequence:

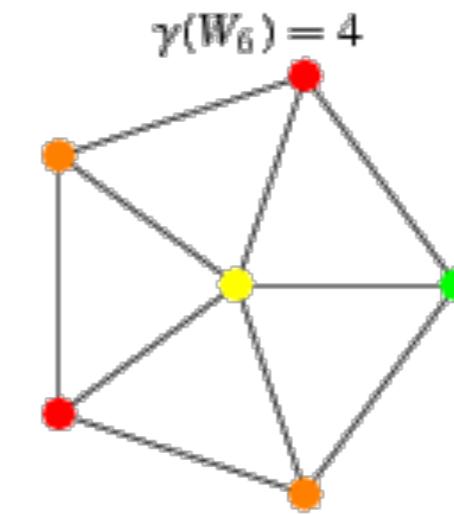
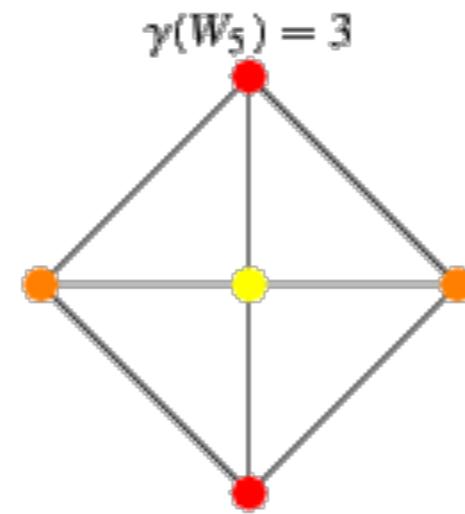
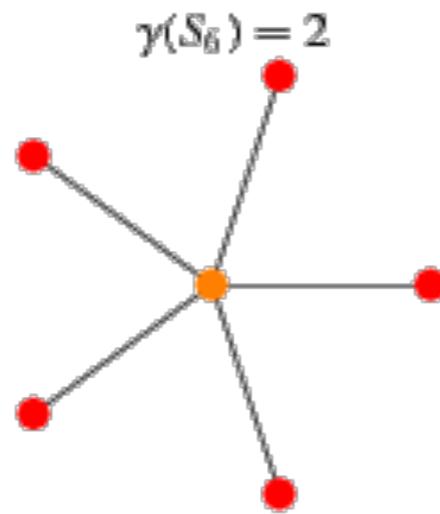
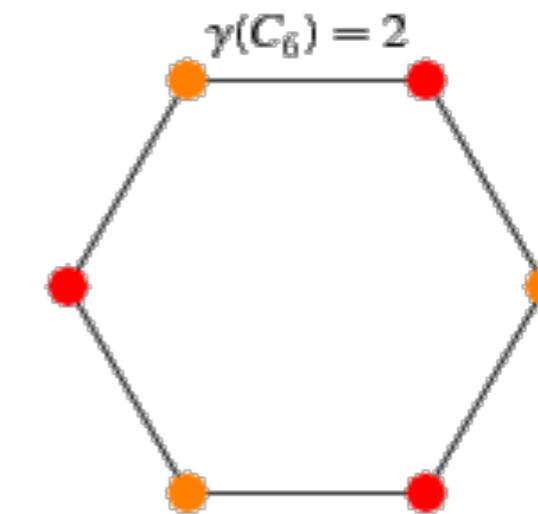
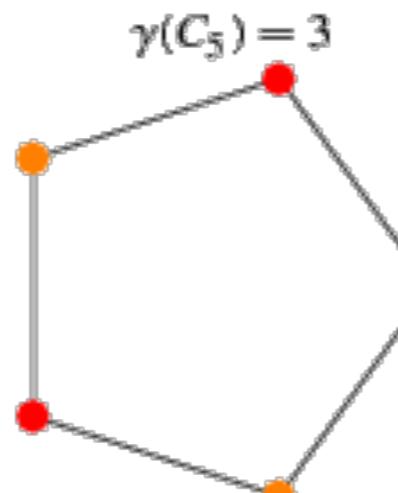
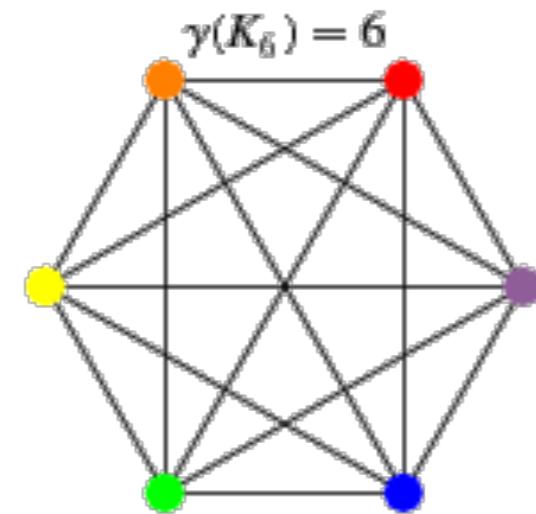
- If G is a **cycle graph** then $L(G)$ and each subsequent graph in this sequence is **isomorphic** to G itself. These are the only connected graphs for which $L(G)$ is isomorphic to G .
- If G is a claw $K_{1,3}$, then $L(G)$ and all subsequent graphs in the sequence are triangles.
- If G is a **path graph** then each subsequent graph in the sequence is a shorter path until eventually the sequence terminates with an **empty graph**.
- In all remaining cases, the sizes of the graphs in this sequence eventually increase without bound.



If G is not connected, this classification applies separately to each component of G .

Chromatic number

smallest number of colors needed to color the vertices of G so that no two adjacent vertices share the same color

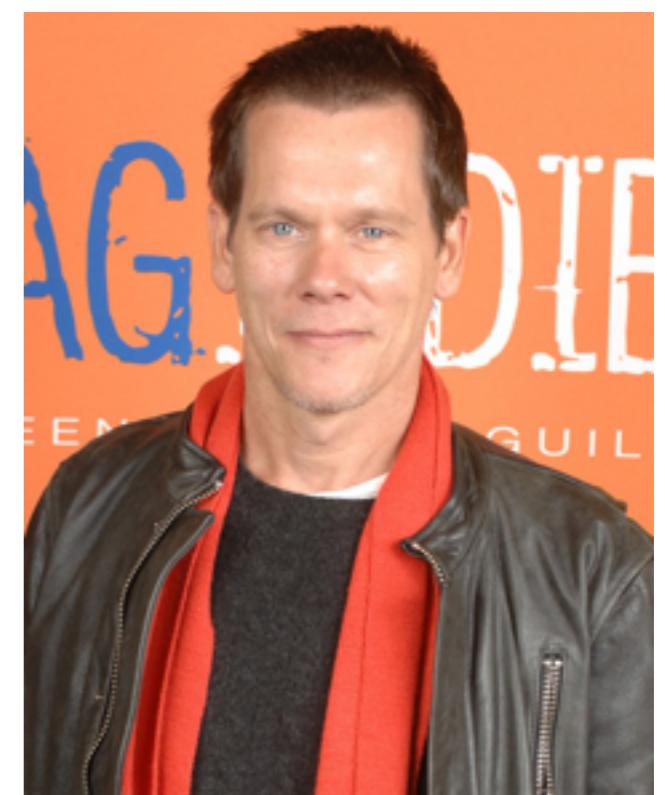
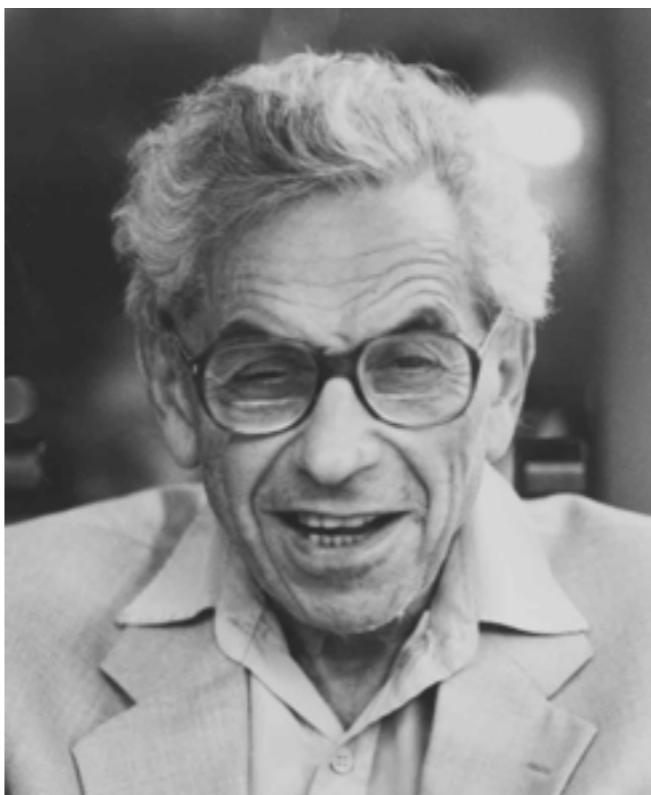


Small-world networks

mean distance between nodes scales as

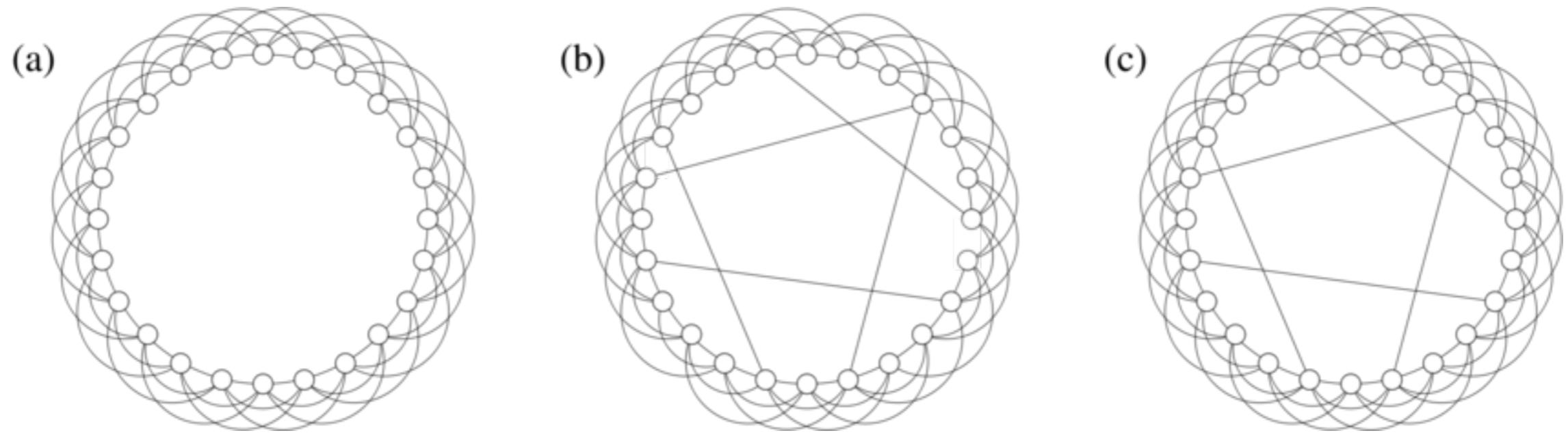
$$D \propto \log |V| \quad |V| \rightarrow \infty$$

- Milgram experiment (1967, 1969)
 - 96 packages from Mass to Omaha
 - target received 18 packages
 - average path length 5.9 ... “6 degrees of separation”
- Erdős number graphs
- Bacon number
- certain protein networks



Watts-Strogatz model

D. J. Watts, S. H. Strogatz. Collective dynamics of *small-world* networks. *Nature* **393**(1), 440–442 (1998)



(a) **Ring network**: each node is connected to the same number $k=3$ nearest neighbors on each side

(b) **Watts-Strogatz** network created by removing each edge with uniform, independent probability p and rewiring it to yield an edge between a pair of nodes that are chosen uniformly at random (avoiding looping and node-replication).

(c) **Newman-Watts** variant of a Watts-Strogatz network, in which one adds "shortcut" edges between pairs of nodes in the same way as in a WS network but without removing edges from the underlying lattice.

Scale-free networks

degree distribution

$$P(k) \propto k^{-\gamma}$$



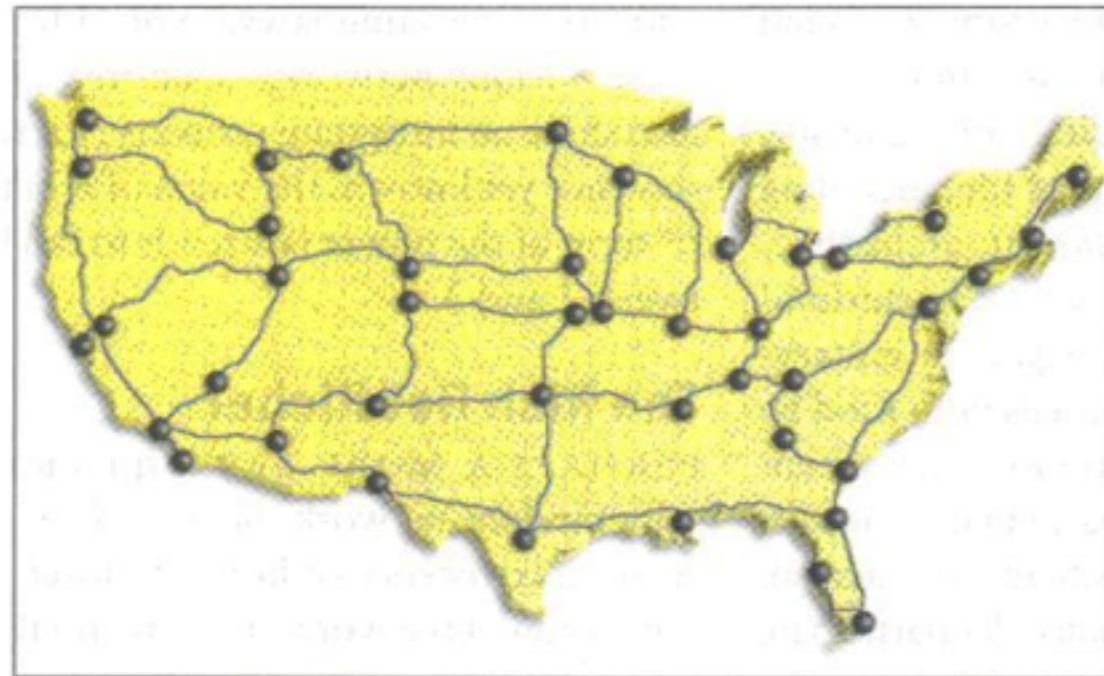
RANDOM VERSUS SCALE-FREE NETWORKS

RANDOM NETWORKS, which resemble the U.S. highway system (*simplified in left map*), consist of nodes with randomly placed connections. In such systems, a plot of the distribution of node linkages will follow a bell-shaped curve (*left graph*), with most nodes having approximately the same number of links.

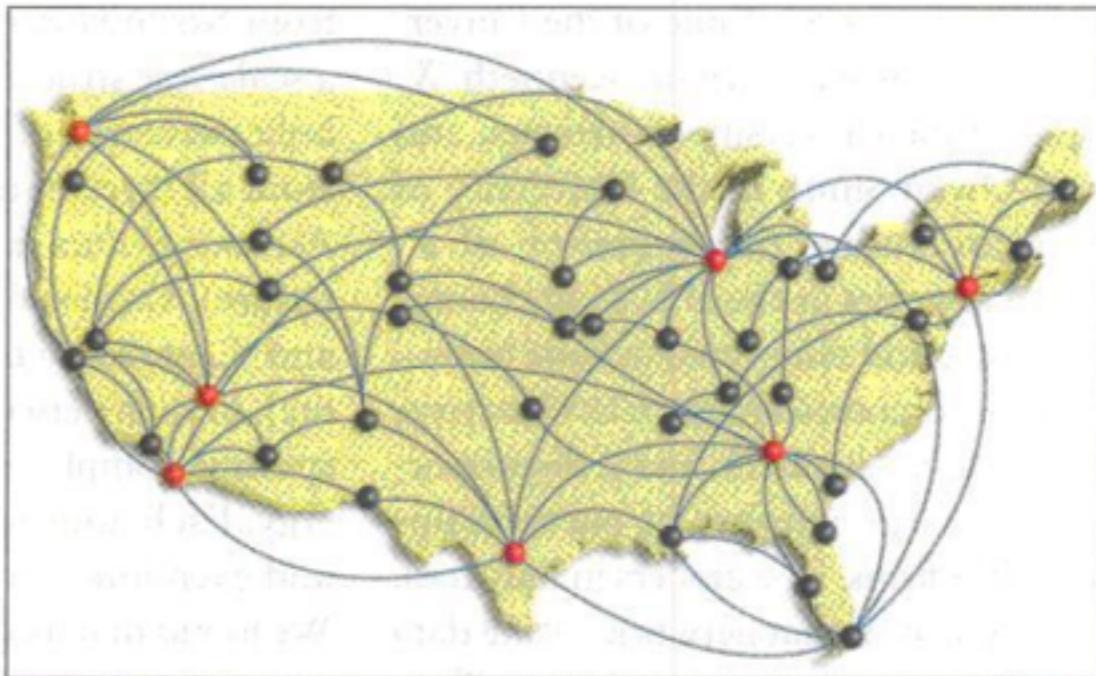
In contrast, scale-free networks, which resemble the U.S. airline system (*simplified in right map*), contain hubs (*red*)—

nodes with a very high number of links. In such networks, the distribution of node linkages follows a power law (*center graph*) in that most nodes have just a few connections and some have a tremendous number of links. In that sense, the system has no "scale." The defining characteristic of such networks is that the distribution of links, if plotted on a double-logarithmic scale (*right graph*), results in a straight line.

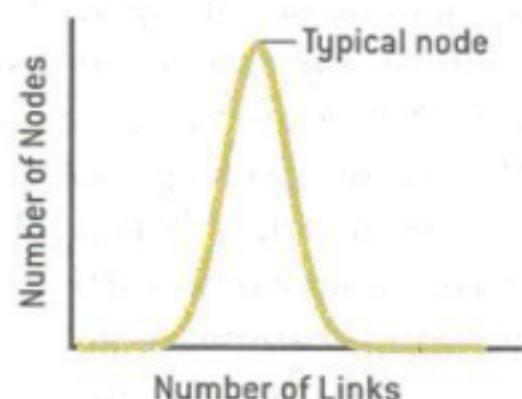
Random Network



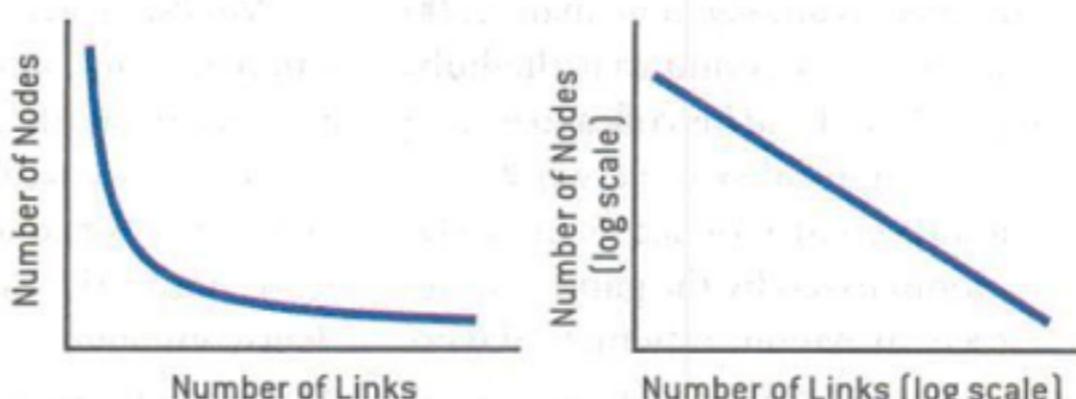
Scale-Free Network



Bell Curve Distribution of Node Linkages



Power Law Distribution of Node Linkages



Examples of Scale-Free Networks

NETWORK	NODES	LINKS
Cellular metabolism	Molecules involved in burning food for energy	Participation in the same biochemical reaction
Hollywood	Actors	Appearance in the same movie
Internet	Routers	Optical and other physical connections
Protein regulatory network	Proteins that help to regulate a cell's activities	Interactions among proteins
Research collaborations	Scientists	Co-authorship of papers
Sexual relationships	People	Sexual contact
World Wide Web	Web pages	URLs

Barabasi & Bonabeau