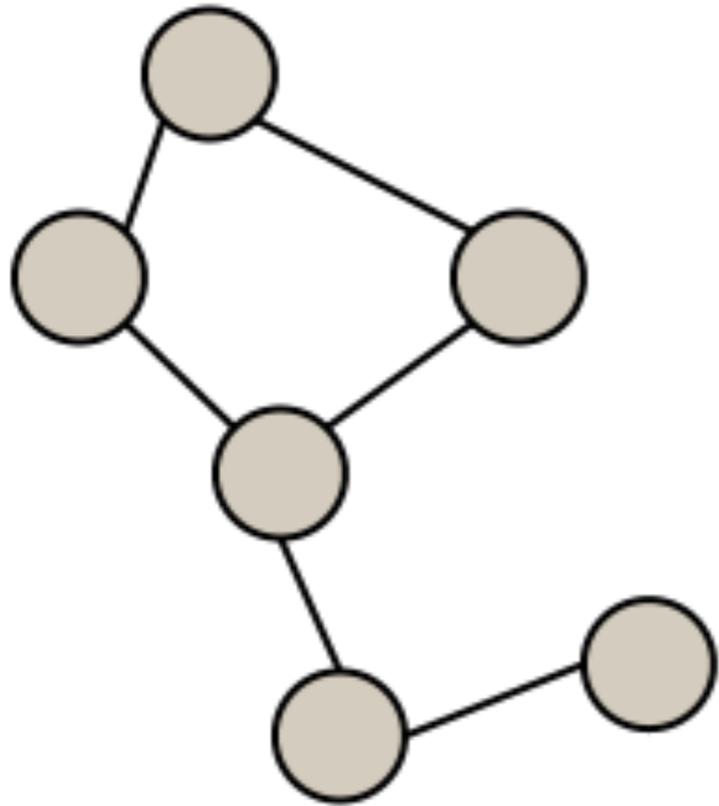


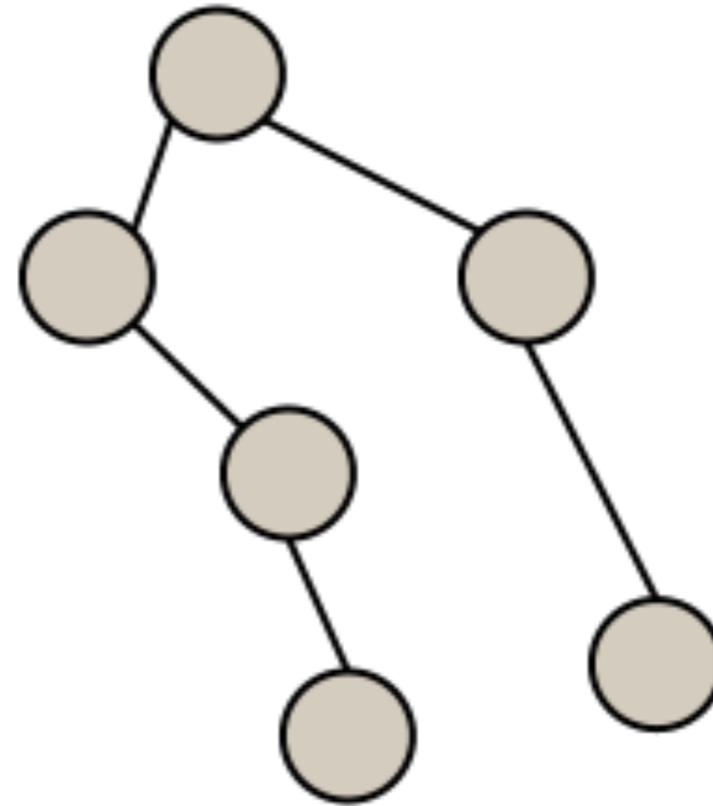
# Basic graph theory

18.S995 - L19

# Graphs & Trees



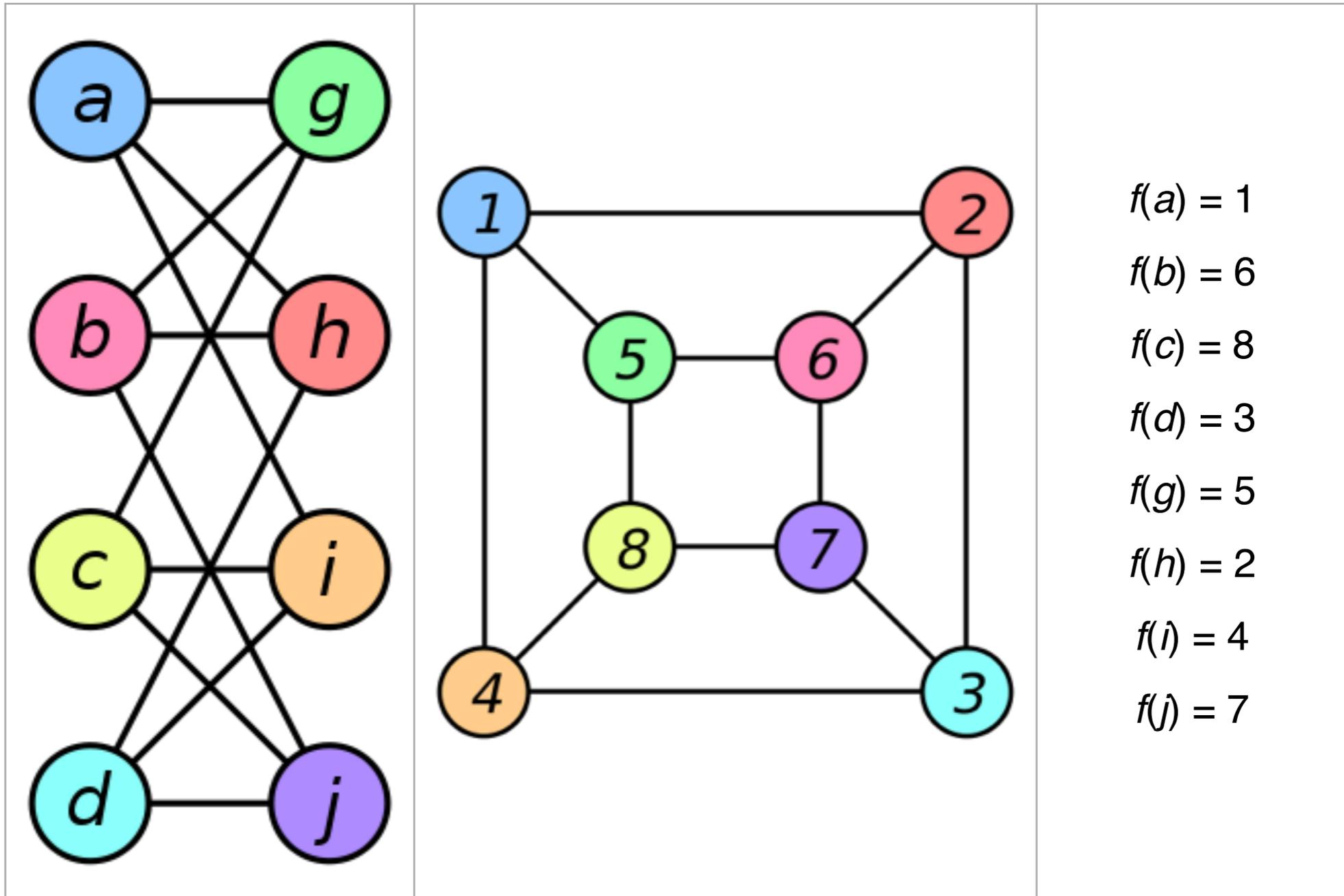
Graph



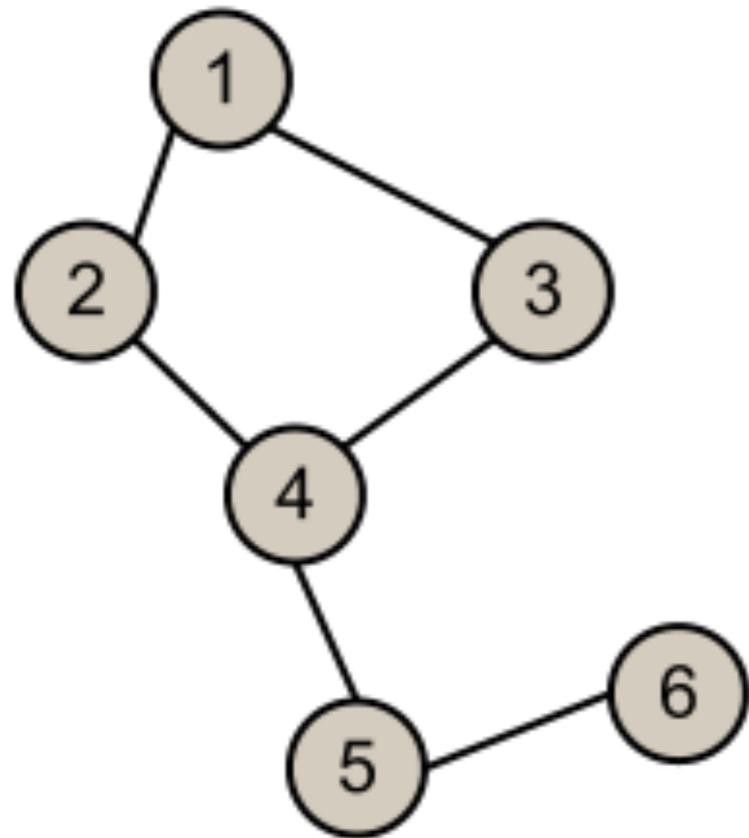
Tree

no cycles

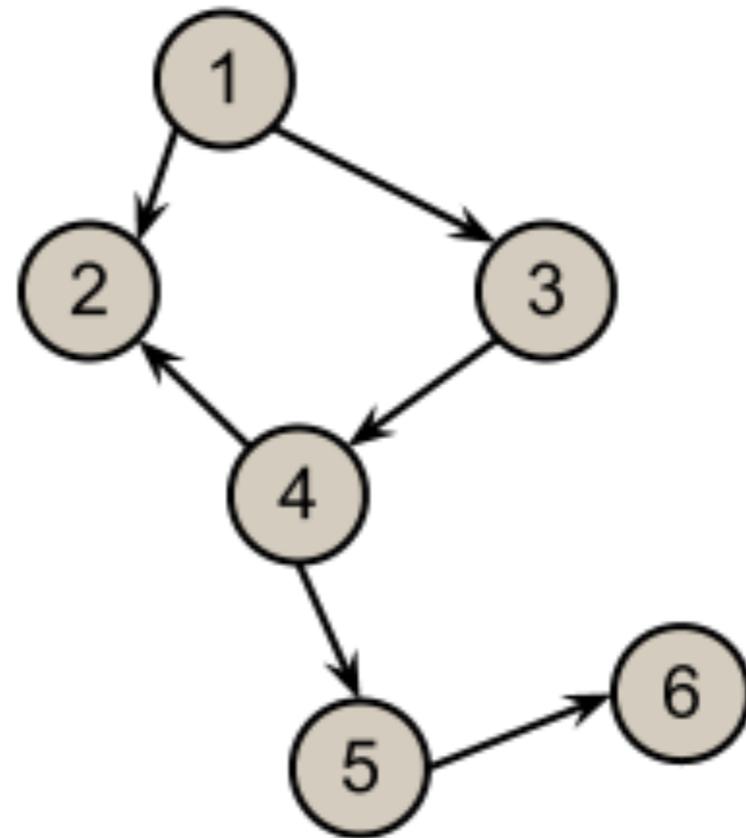
# Isomorphic graphs



# Directed Graph

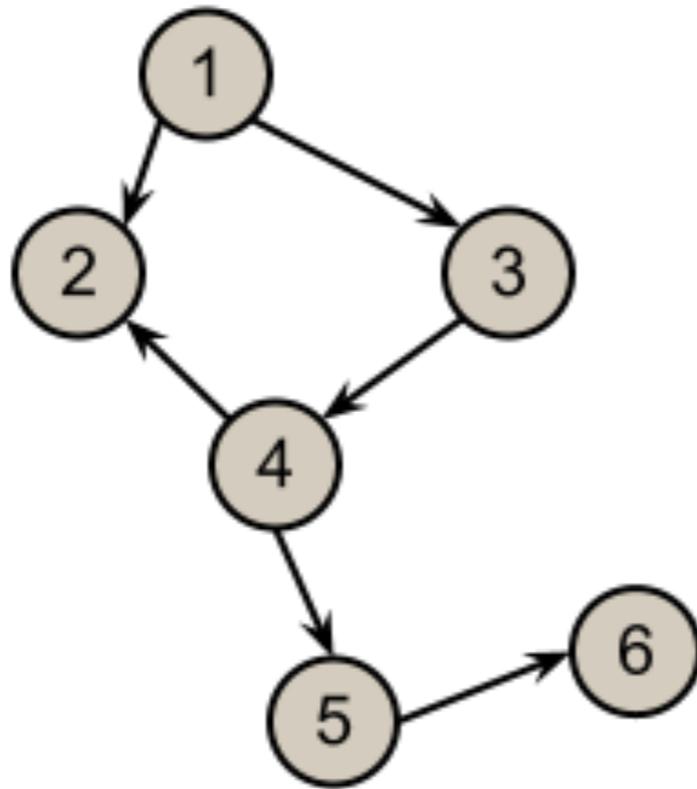


Undirected

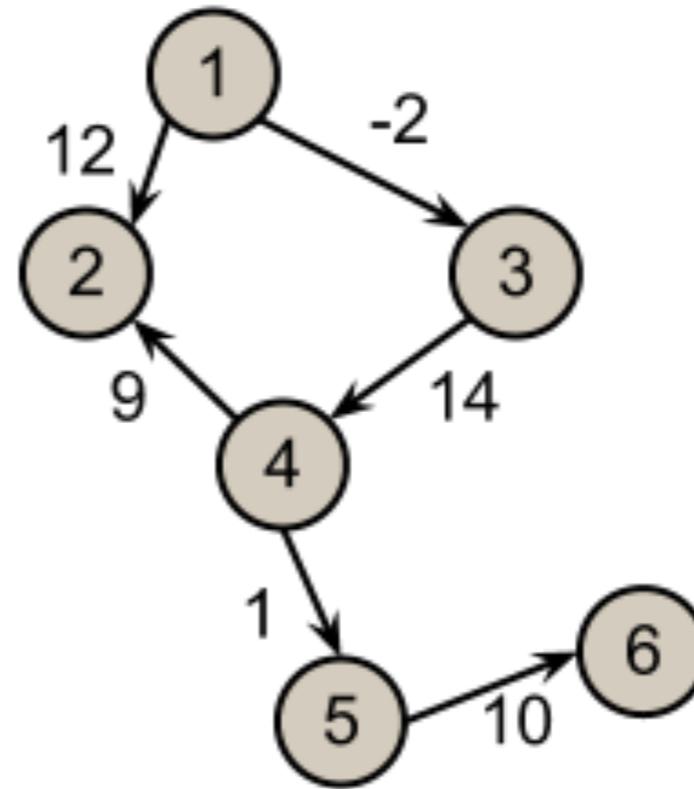


Directed

# Weighted Graph

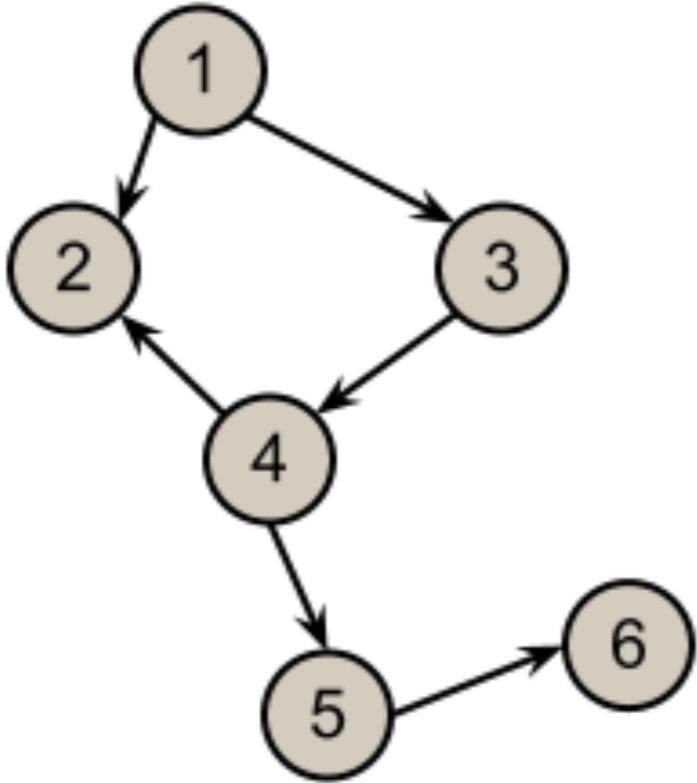


Unweighted

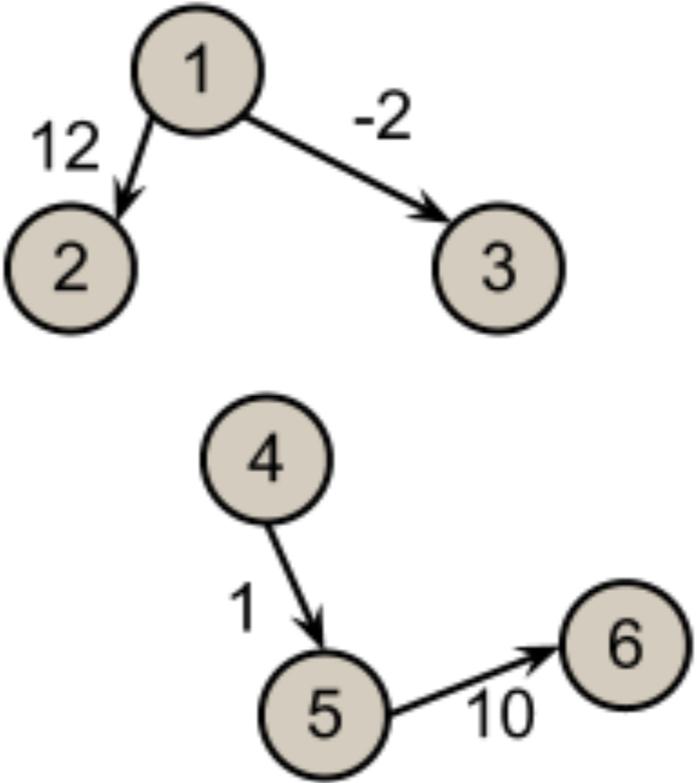


Weighted

# Connected Graph

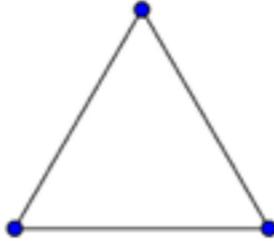
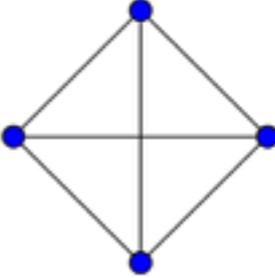
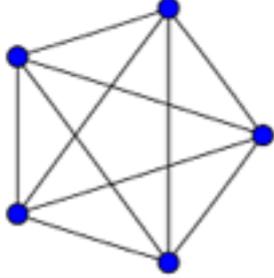
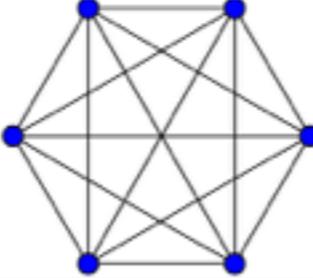
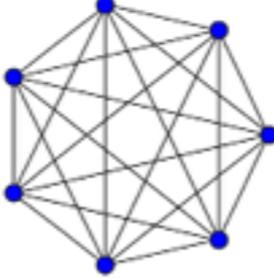
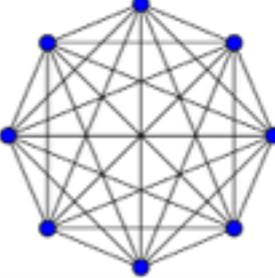
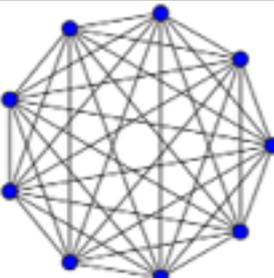
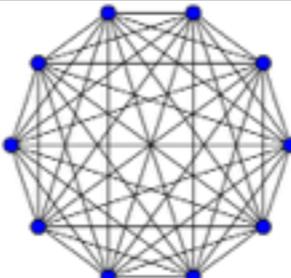
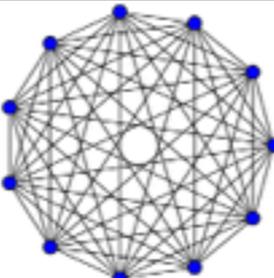
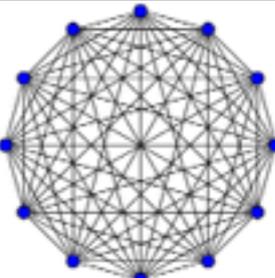


Connected

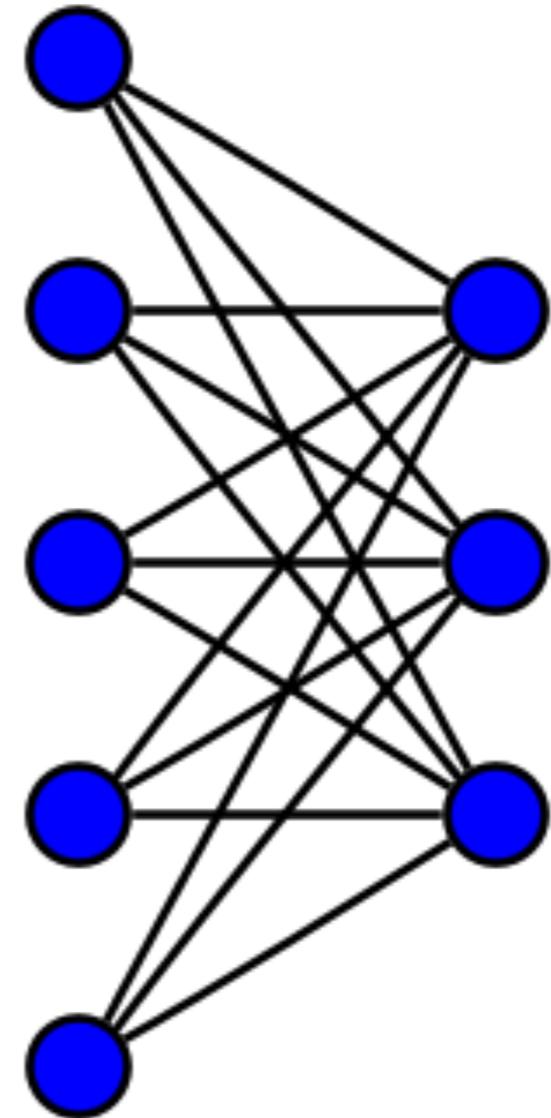
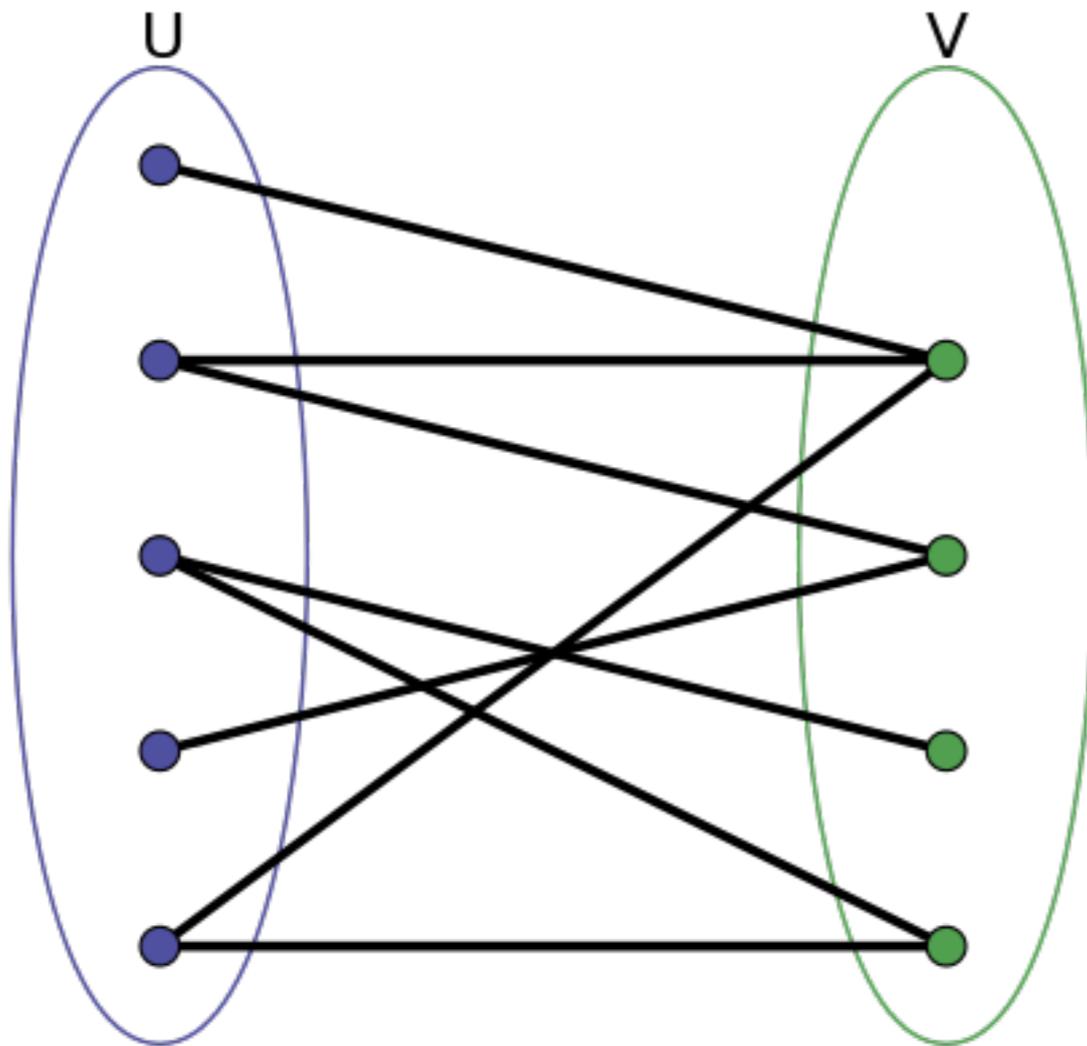


Disconnected

# 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

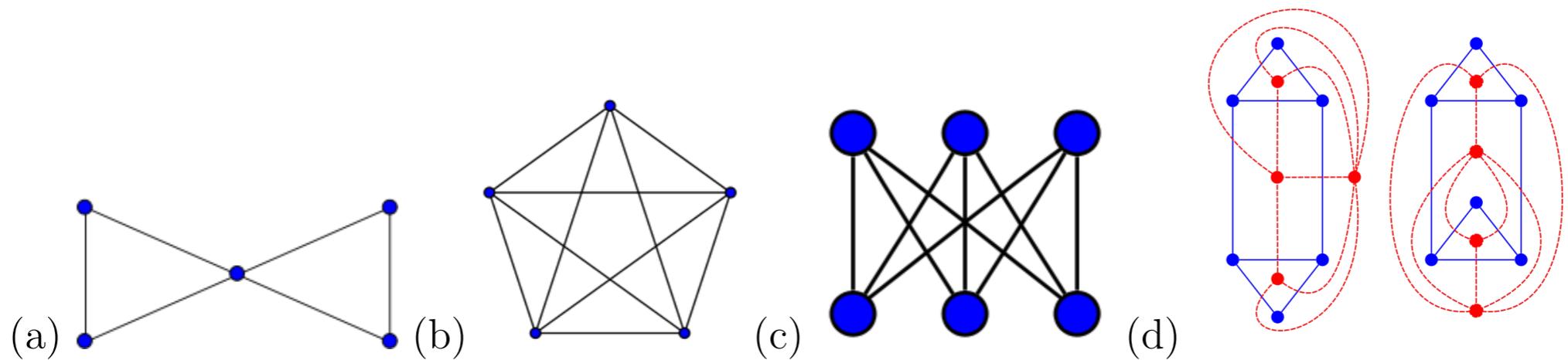
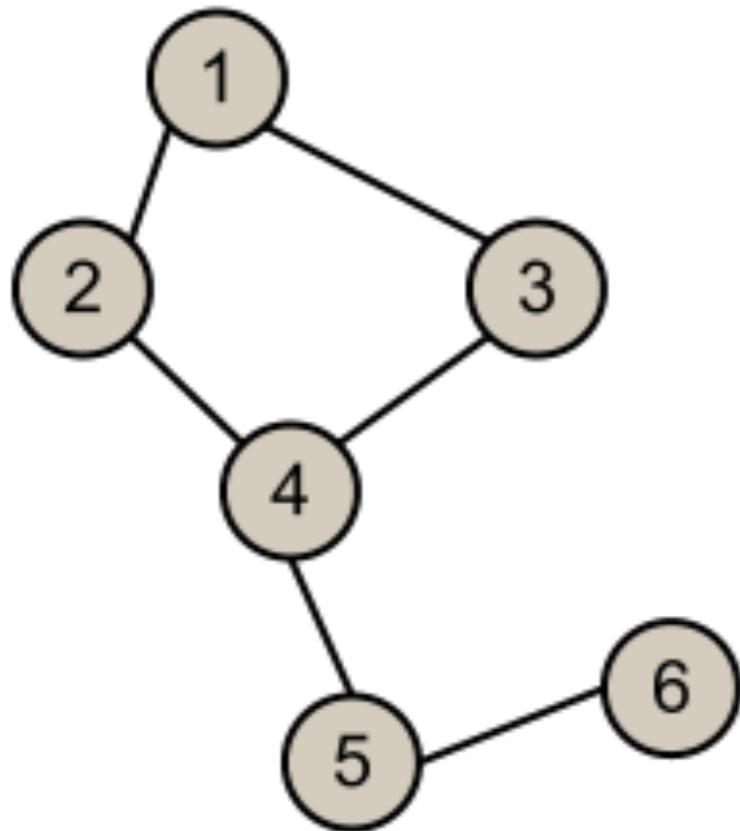


Figure 1.2: Planar, non-planar and dual graphs. (a) Plane ‘butterfly’ graph. (b, c) Non-planar graphs. (d) The two red graphs are both dual to the blue graph but they are not isomorphic. Image source: wiki.

Algebraic characterization

# Undirected Graph & Adjacency Matrix



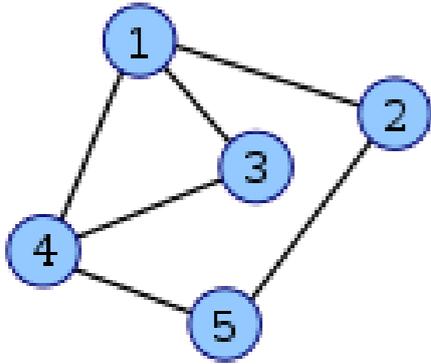
Undirected Graph

	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

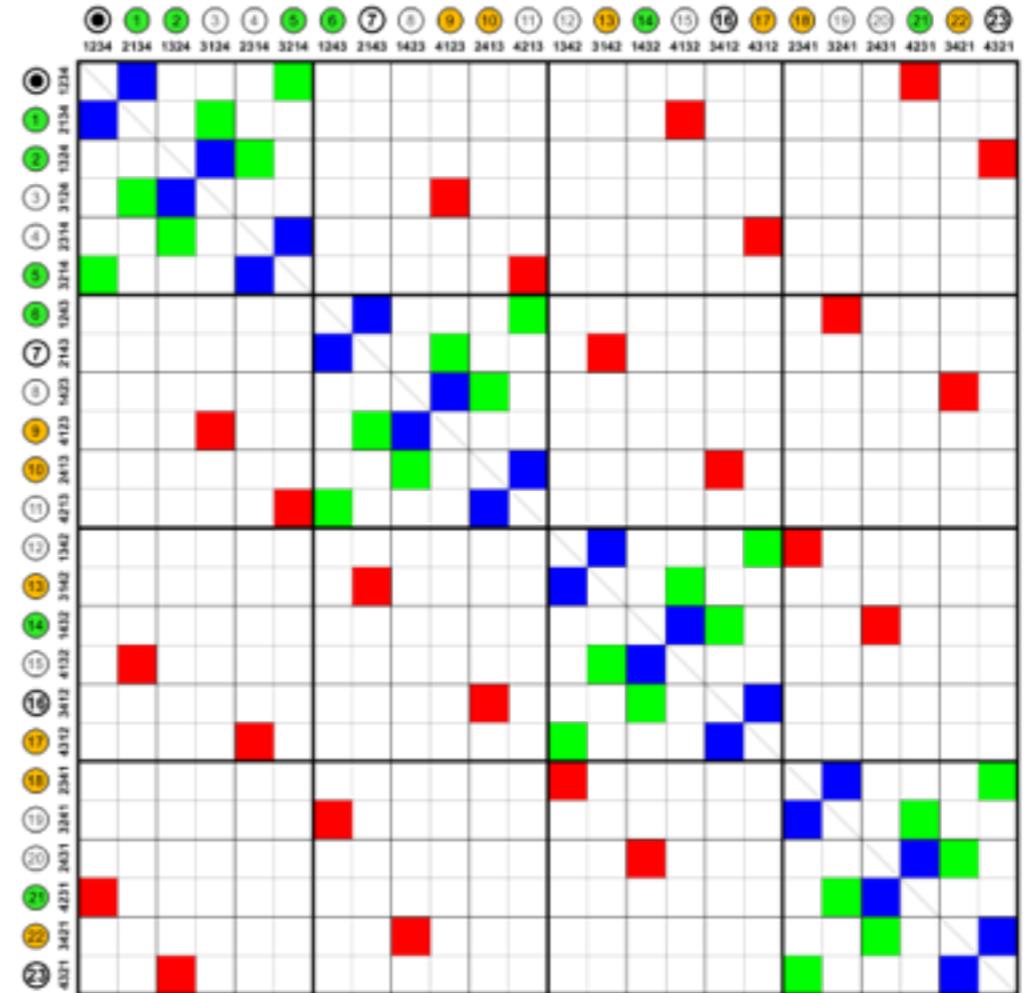
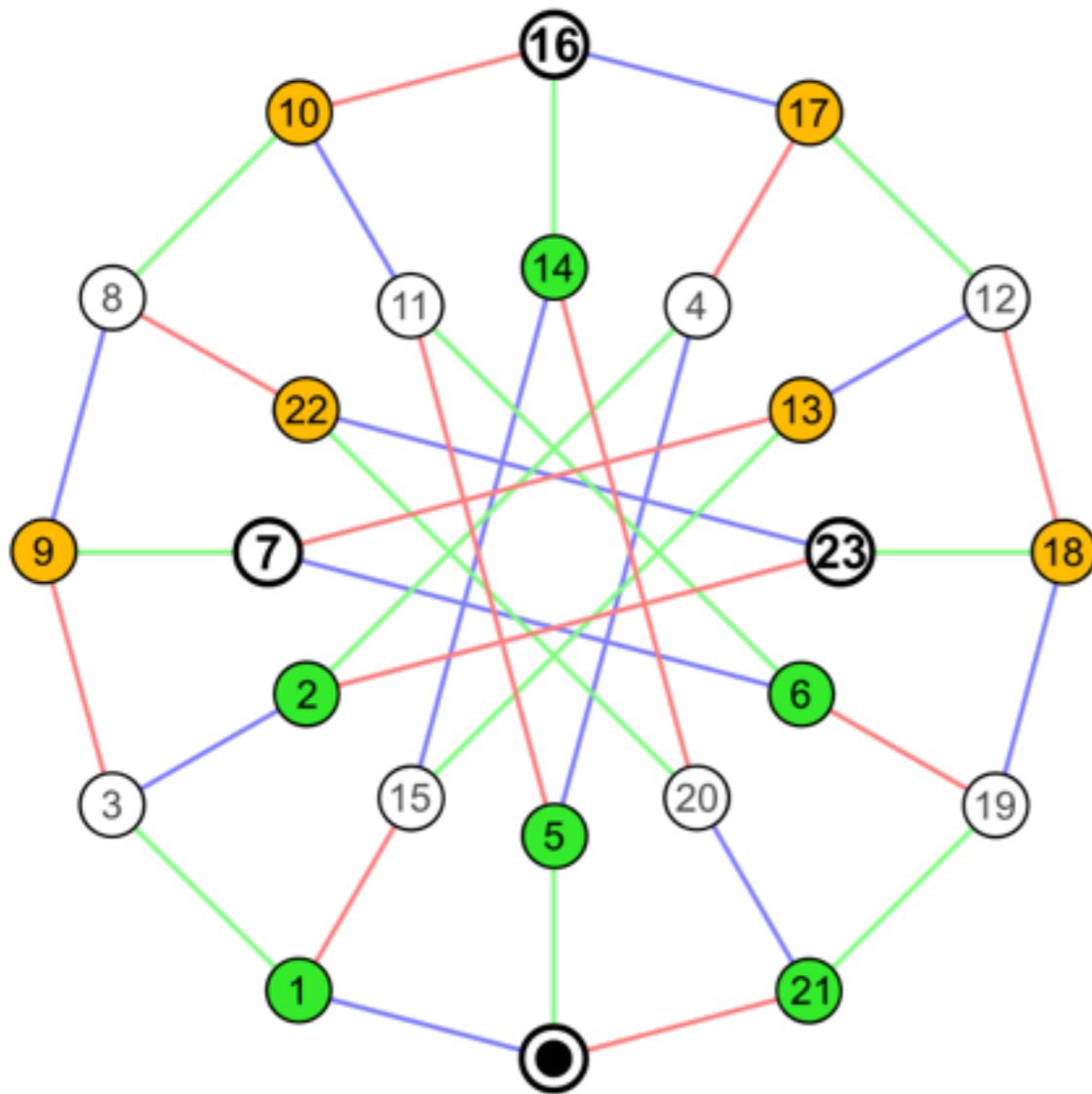
$$p(\mathcal{G}; x) = \det(\mathbf{A} - x\mathbf{I}) \quad (1.7)$$

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

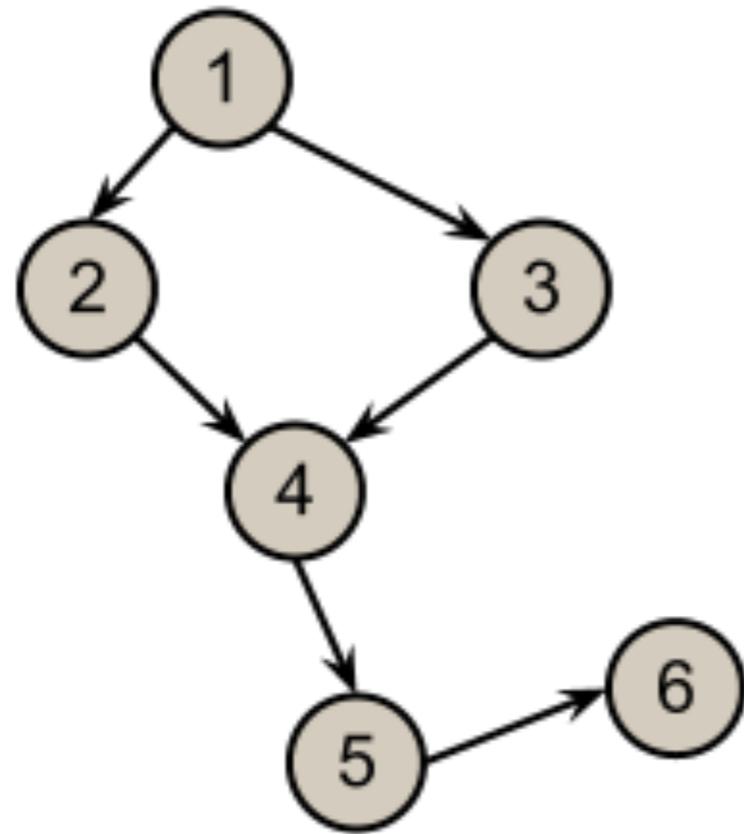


Nauru graph

“integer graph”

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

# Directed Graph & Adjacency Matrix



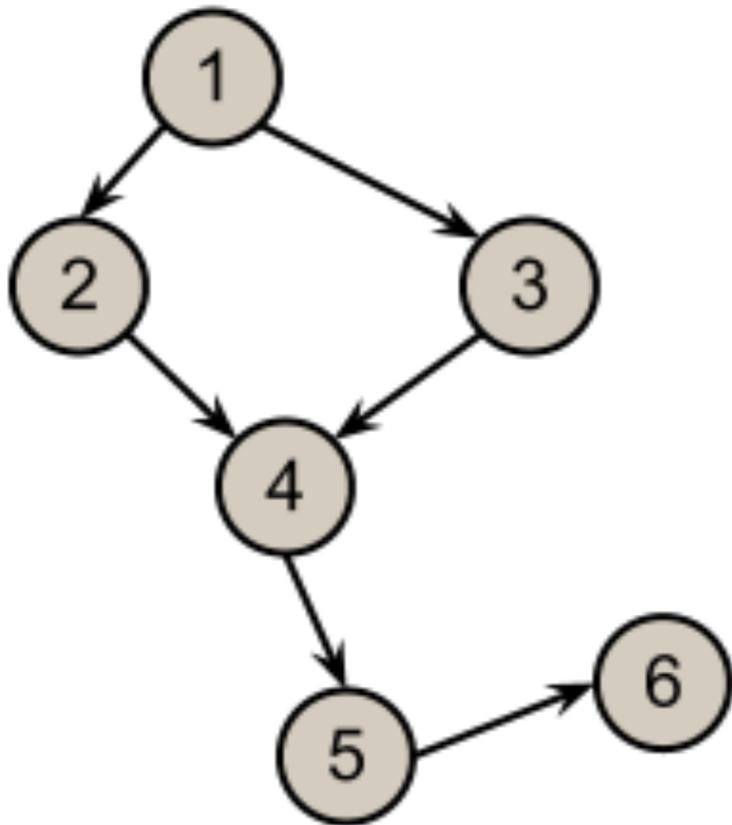
Undirected Graph

	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

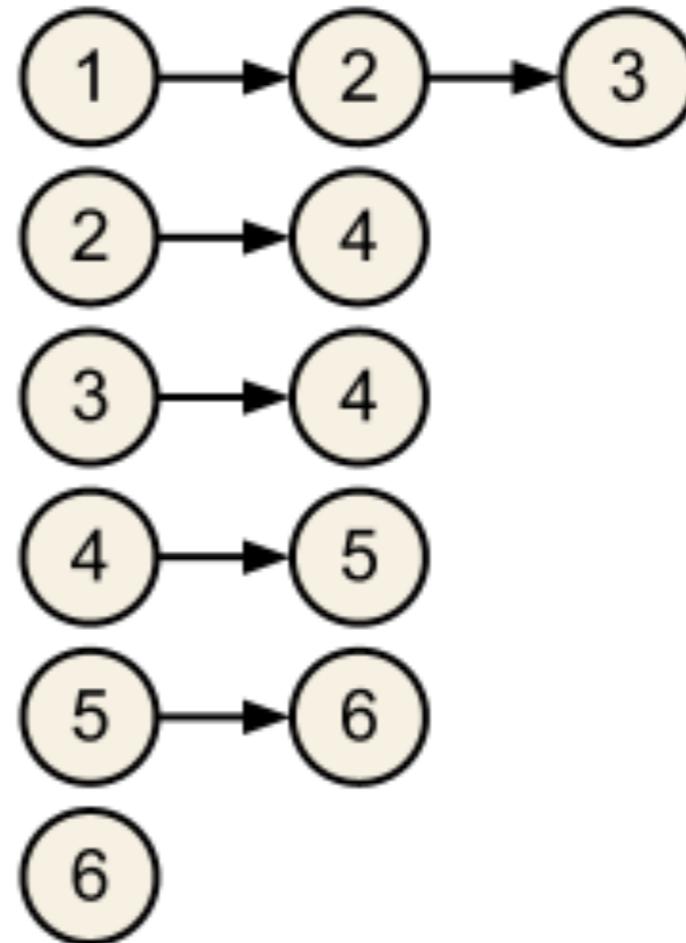
Adjacency Matrix

$|V| \times |V|$  matrix

# Directed Graph & Adjacency List



Undirected Graph



Adjacency List

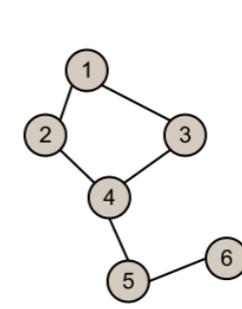
# Complexity

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

# Complexity

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

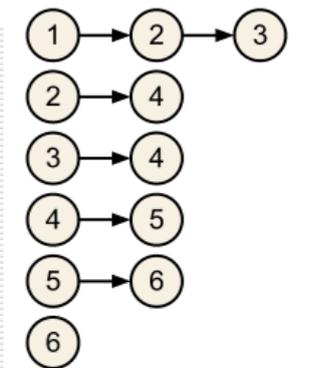
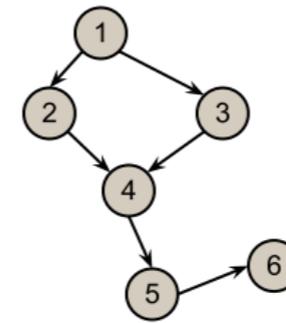
Adjacency Matrix

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

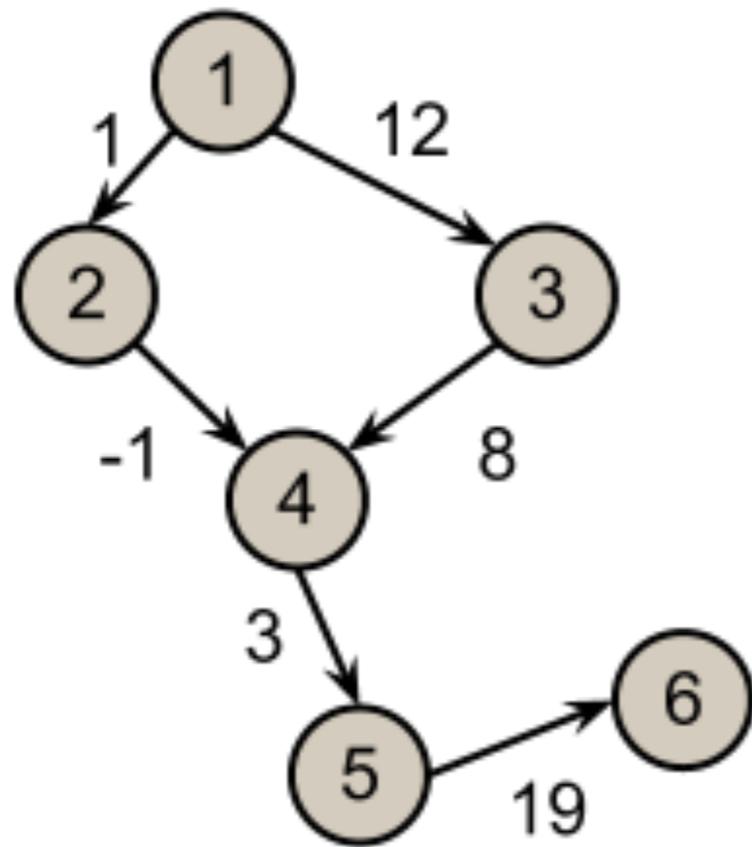
Directed Graph & Adjacency List



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

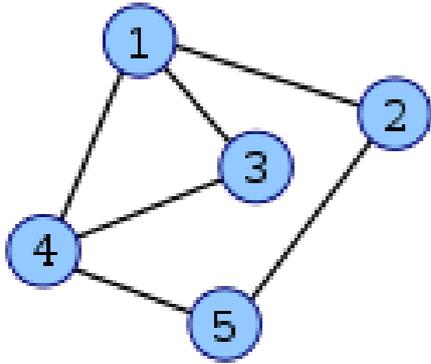


Weighted Directed Graph

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

Adjacency Matrix

# Degree matrix



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

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

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

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

For the graph in Fig. 1.3a, one has

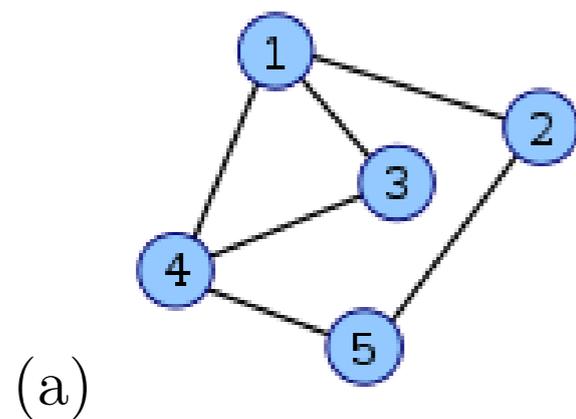
$$\mathbf{D} = \begin{pmatrix} 3 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{pmatrix} \quad (1.5)$$

**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

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

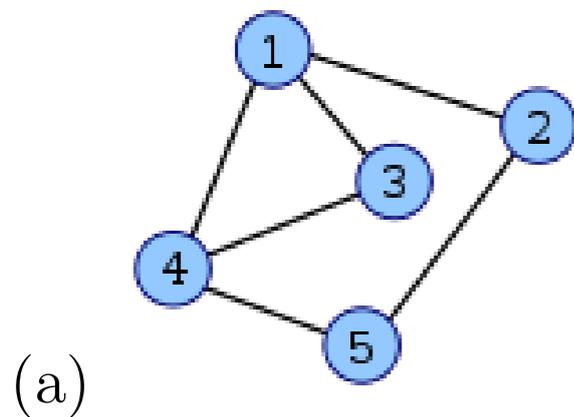
Hence

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

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

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



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

**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

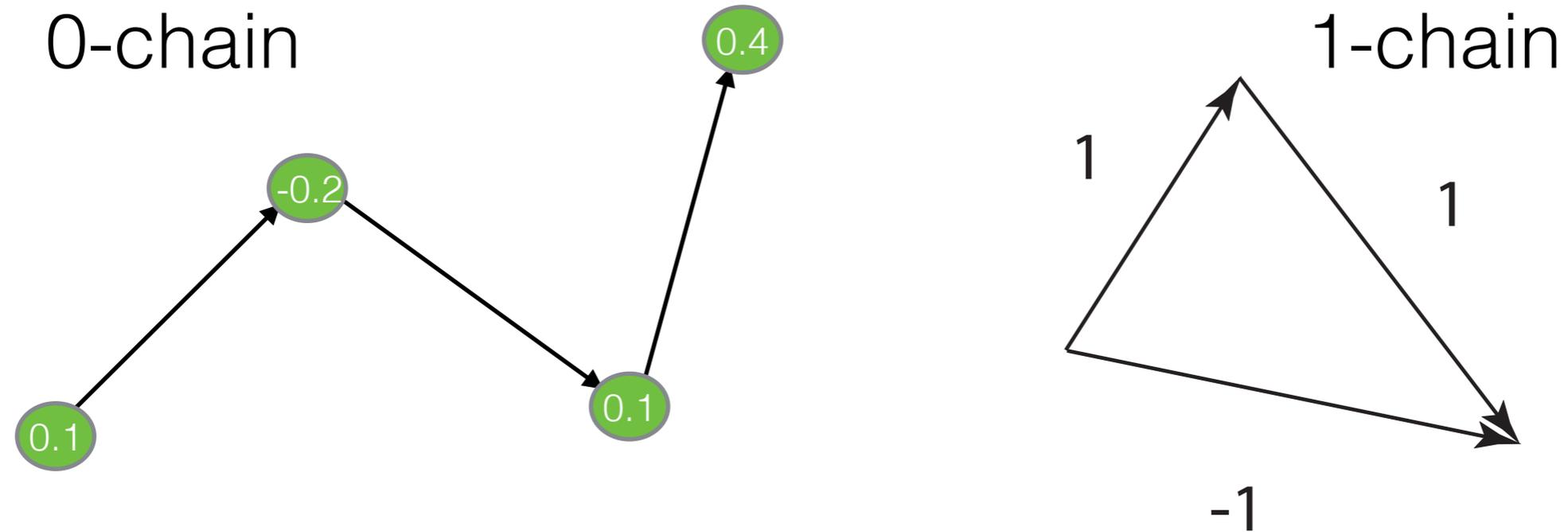
$$\bar{L}_{ij} = \begin{cases} 1, & \text{if } i = j \text{ and } \deg(v_i) \neq 0 \\ -1/\sqrt{\deg(v_i) \deg(v_j)}, & \text{if } i \neq j \text{ and } v_i \text{ and } v_j \text{ are connected by edge} \\ 0, & \text{otherwise} \end{cases} \quad (1.19b)$$

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

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



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  $\vec{\mathbf{B}} = (\vec{B}_{is})$  can be viewed as *boundary operator* that maps 1-chains onto 0-chains, while the transposed matrix  $\vec{\mathbf{B}}^\top = (\vec{B}_{si})$  is a *co-boundary operator* that maps 0-chains onto 1-chains. Accordingly  $\bar{\mathbf{L}}$  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  $\bar{\mathbf{L}} \cdot \mathbf{g}$ , such that

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

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

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

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

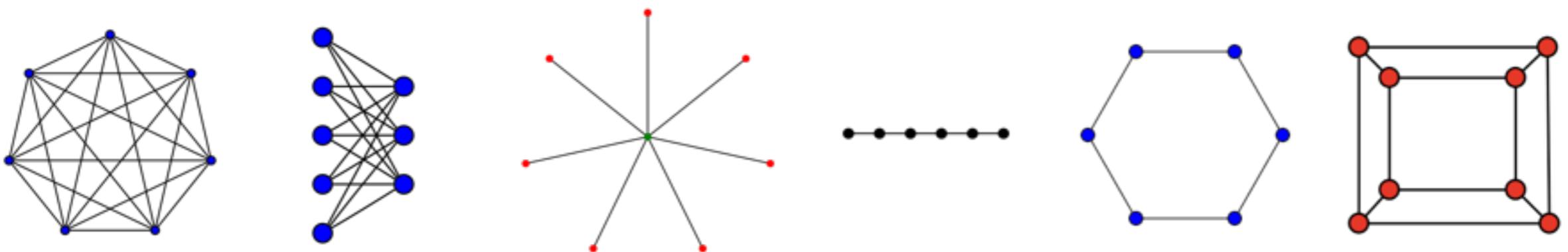
Abbreviating  $n = |V|$ , one can show that

- (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  $k = 0, \dots, n$ .



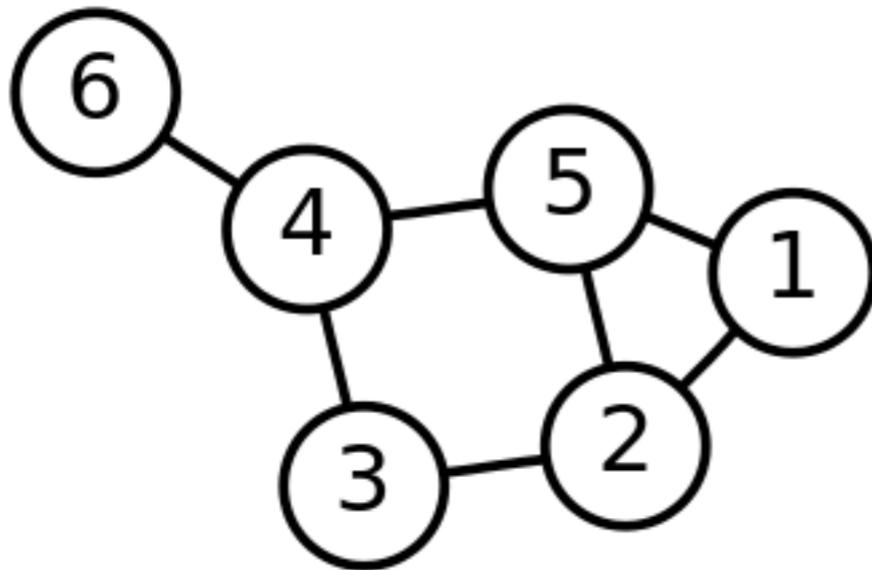
# Graph Laplacian

$$L = D - A$$

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

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

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

$$\lambda_0 \leq \lambda_1 \leq \dots \leq \lambda_{|V|} \tag{1.18}$$

The following properties hold:

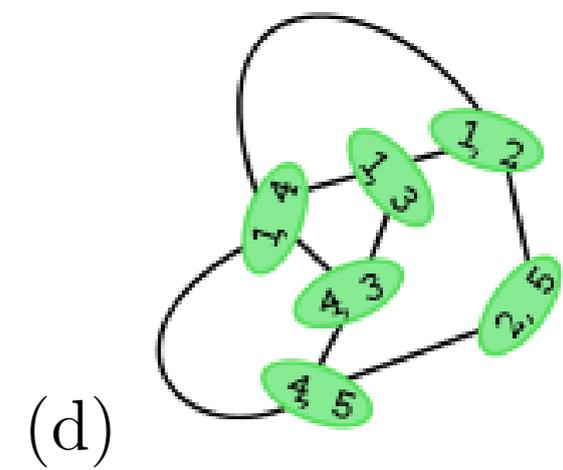
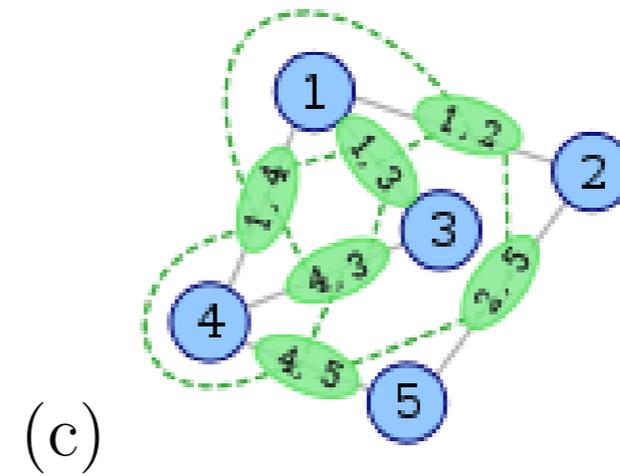
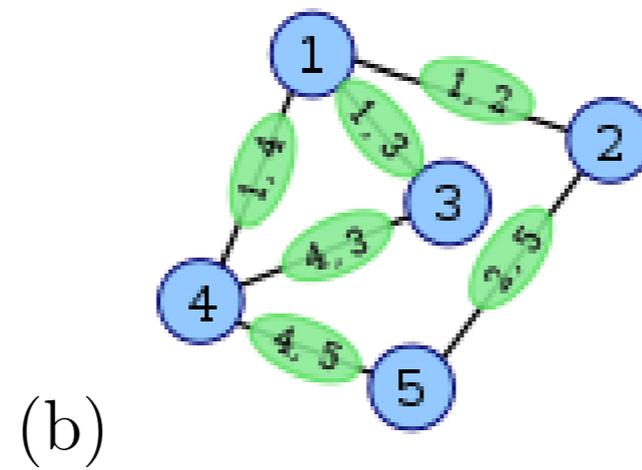
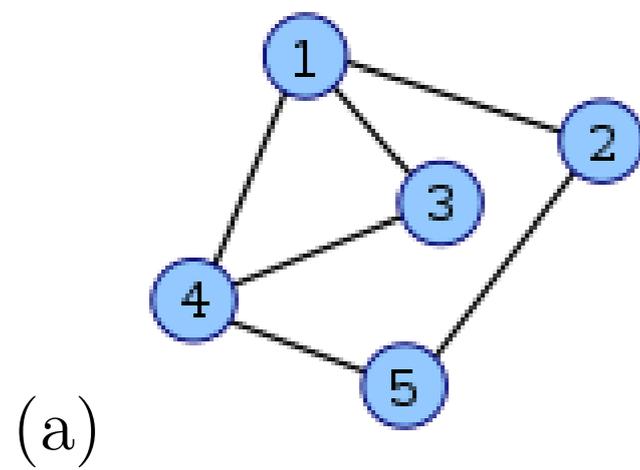
- (i)  $\mathbf{L}$  is symmetric.
- (ii)  $\mathbf{L}$  is positive-semidefinite, that is  $\lambda_i \geq 0$  for all  $i$ .
- (iii) Every row sum and column sum of  $\mathbf{L}$  is zero.<sup>2</sup>
- (iv)  $\lambda_0 = 0$  as the vector  $\mathbf{v}_0 = (1, 1, \dots, 1)$  satisfies  $\mathbf{L} \cdot \mathbf{v}_0 = \mathbf{0}$ .
- (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.

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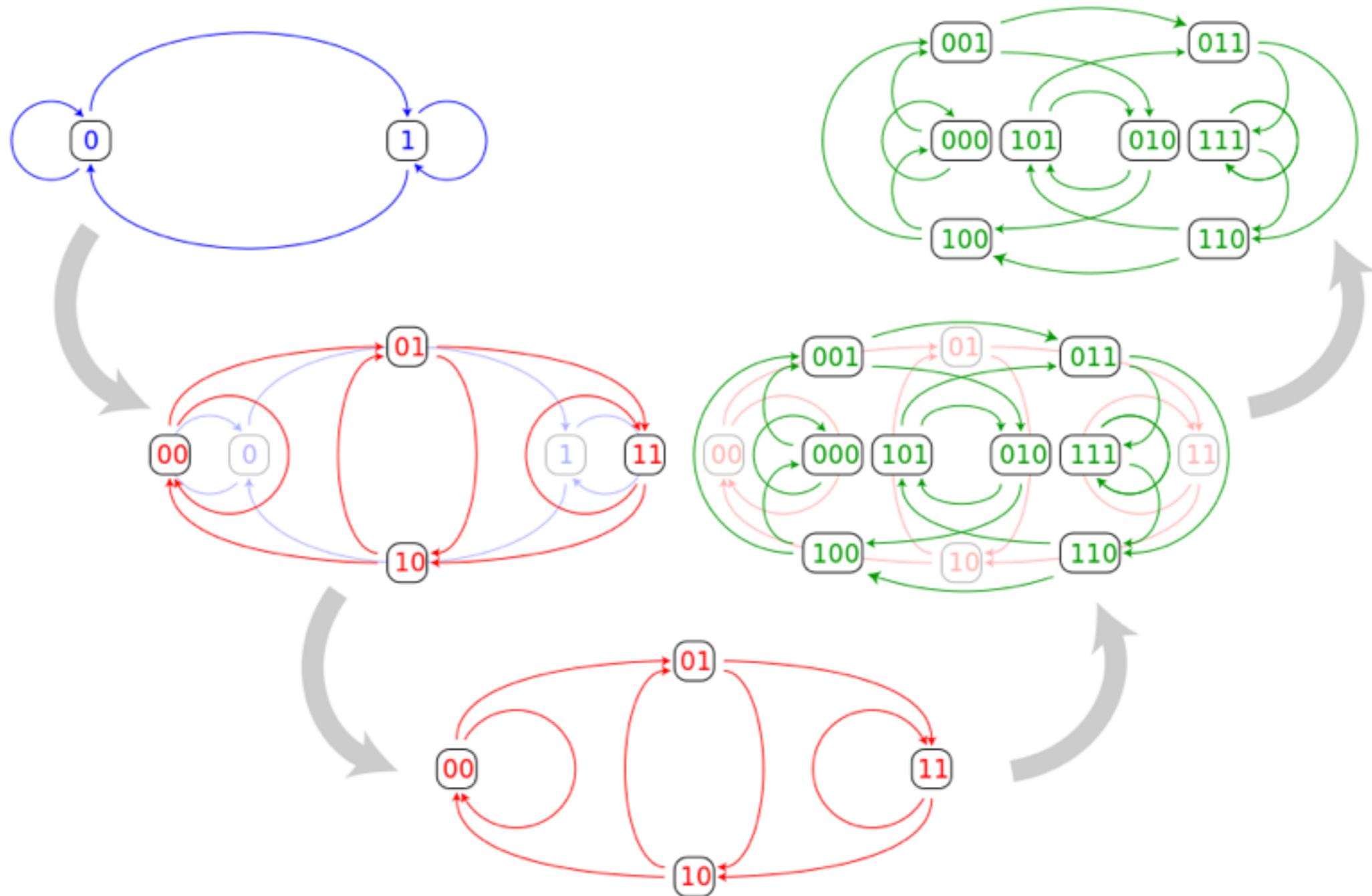
<sup>2</sup>The degree of the vertex is summed with a -1 for each neighbor

# Line graphs of **undirected** graphs

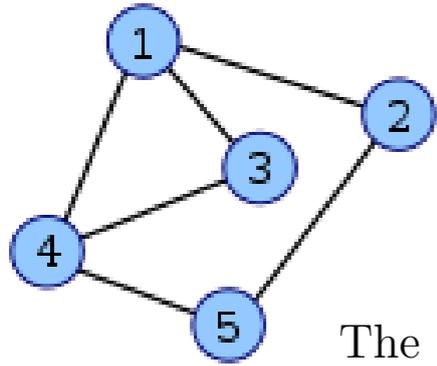
1. draw vertex for each edge in  $G$
2. connect vertices if edges have joint point



# 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



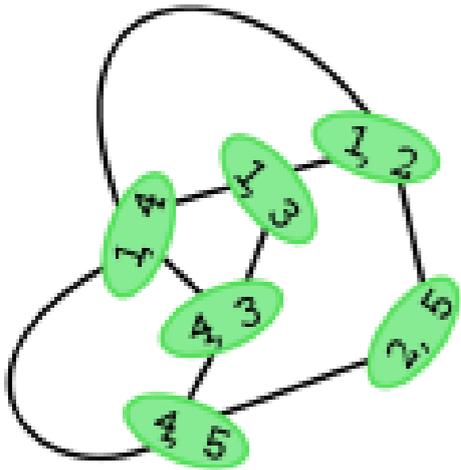
$$\mathbf{C} = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \end{pmatrix} \quad (1.9)$$

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

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

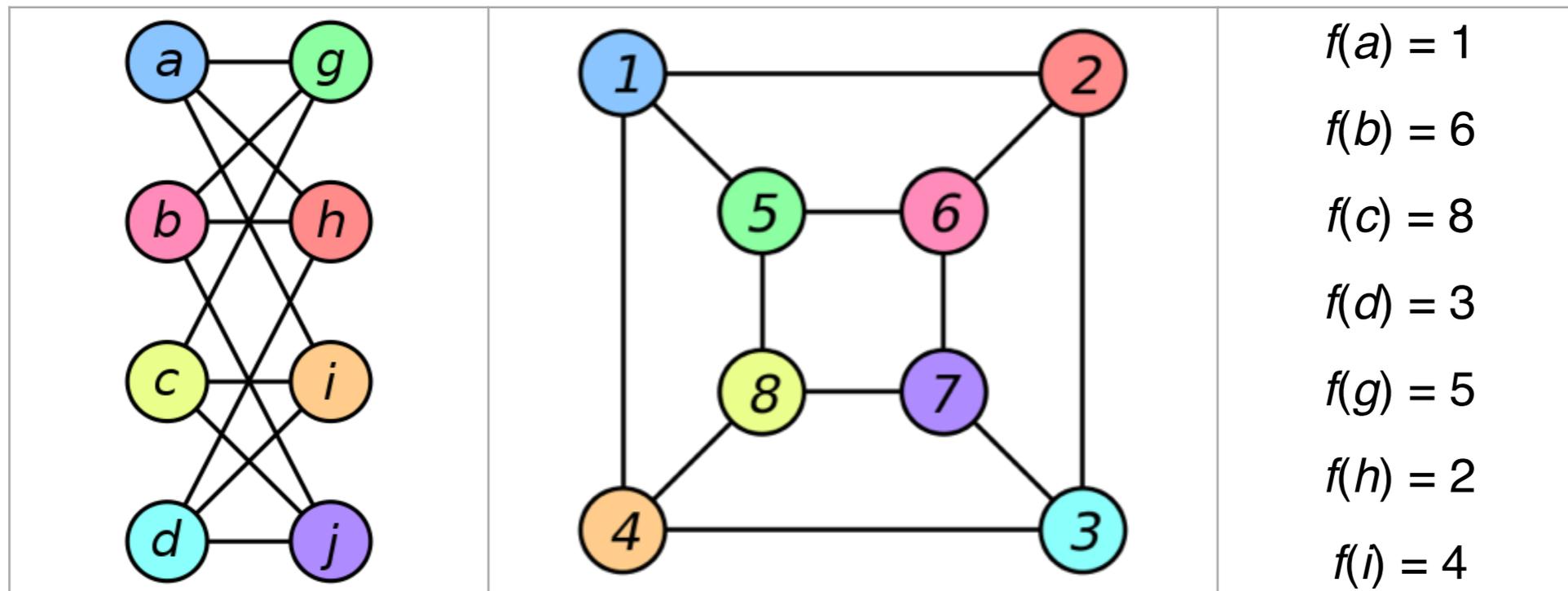


characteristic polynomial

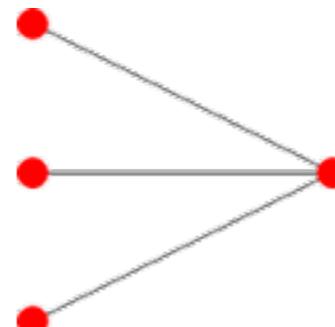
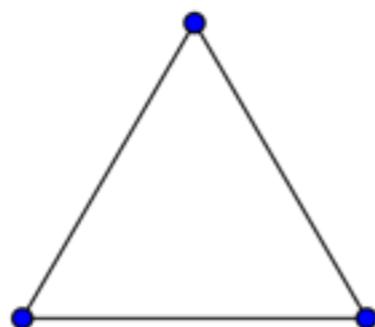
$$p(\mathcal{L}[\mathcal{G}]; x) = (x + 2) (x^2 + x - 1) [(x - 3)x^2 - x + 2]$$

# 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.



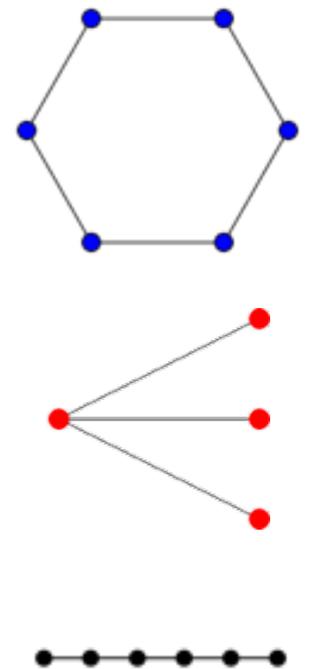
# Line graphs of line graphs of ....

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

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 so that no two adjacent vertices share the same color

