

# Discrete Mathematics: Lecture 20

## Part IV. Graph Theory

graph, vertex, edge, endpoints, directed, undirected, multiple edge, loop,  
complete graph, cycle, wheel, cube, graph representation

Xuming He

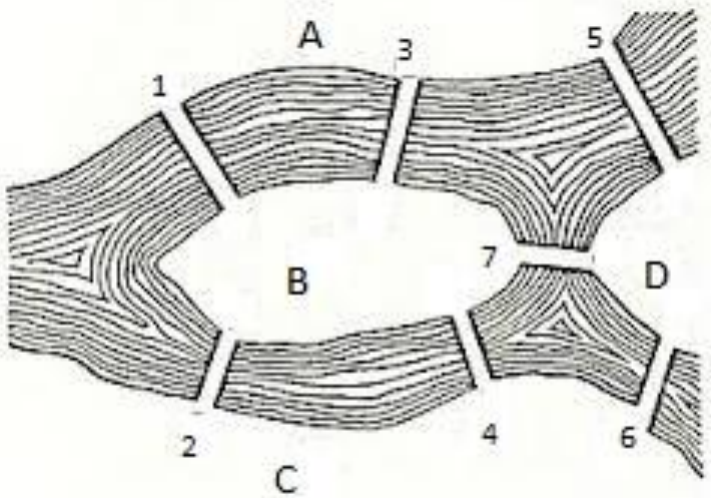
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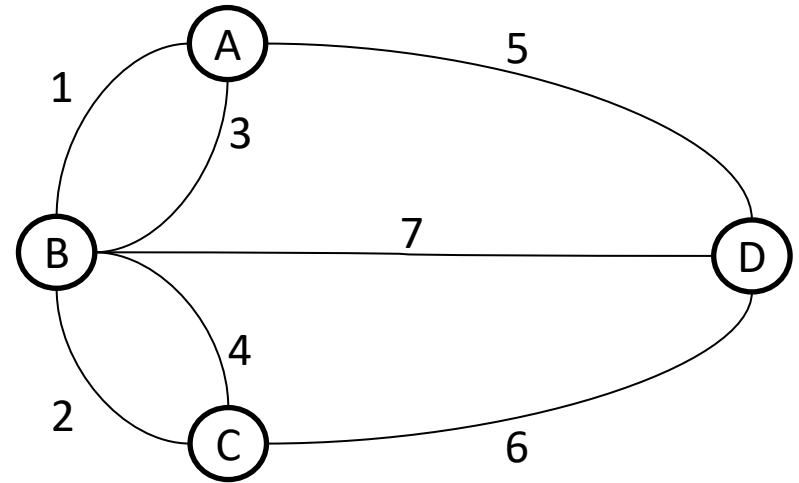
Spring Semester, 2025

Notes by Prof. Liangfeng Zhang and Xuming He

# Seven Bridges of Königsberg



*The Königsberg Bridges.*



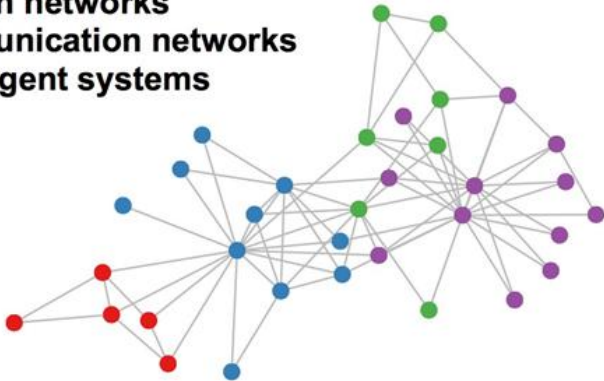
**QUESTION:** Is it possible to travel all seven bridges without repetition?

- Start at one of the four locations  $A, B, C, D$
- Travel across every bridge exactly once
- Return to the starting point

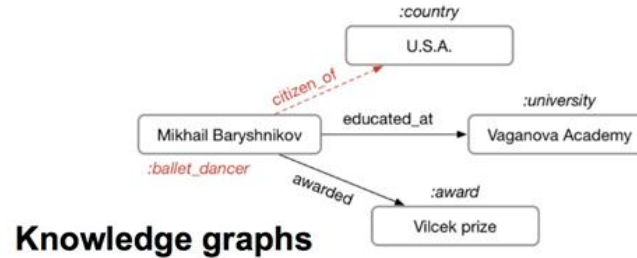
**Graph Notion:** Euler Circuit (1736)

# Real-world Graphs

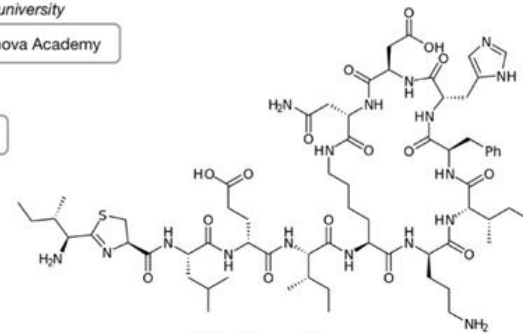
**Social networks**  
**Citation networks**  
**Communication networks**  
**Multi-agent systems**



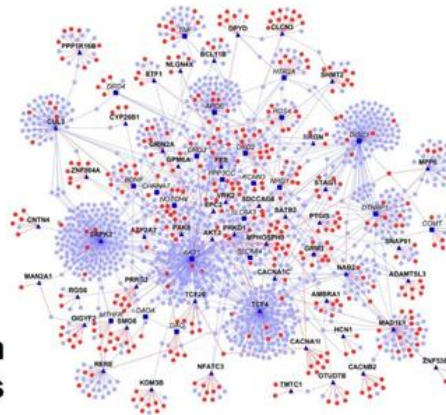
## Protein interaction networks



## Knowledge graphs



## Molecules



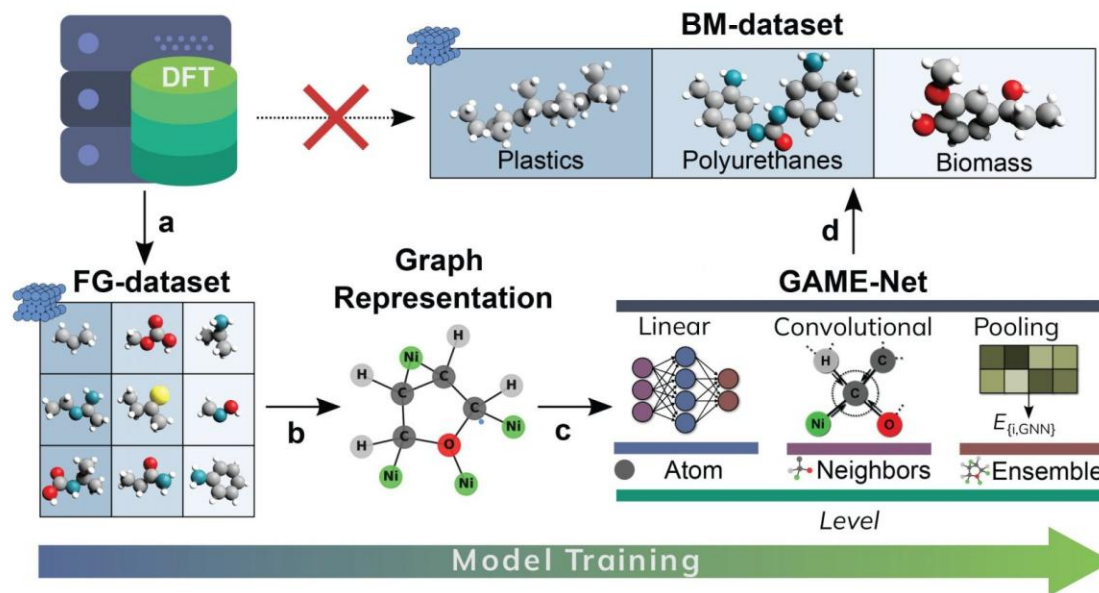
## Road maps



# AI and Graphs

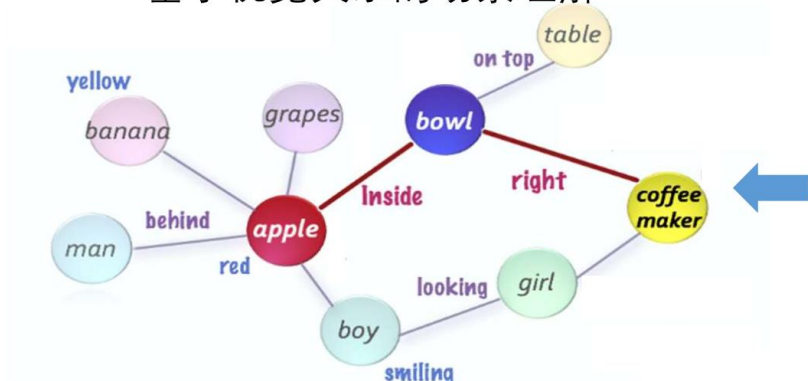
## “Fast Evaluation of the Adsorption Energy of Organic Molecules on Metals via Graph Neural Networks”

*Nature Comp. Sci.* 2023



# AI and Graphs

场景图：  
基于视觉关系的场景理解

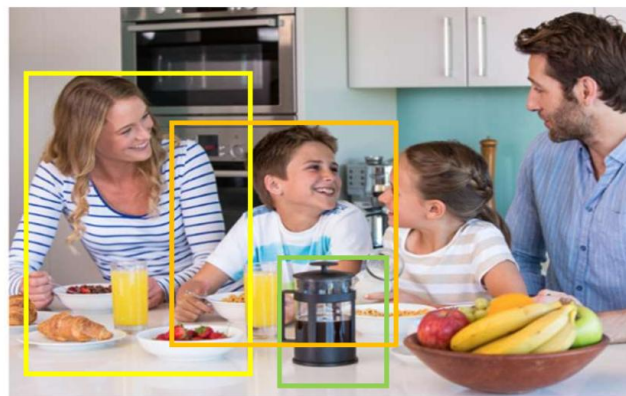


视觉定位

The **female** is **at the left**.  
The **cup** is **next to the coffeemaker**.  
The **male** is **smiling**.

图文匹配

The **boy** is **eating banana**. X  
The **boy** is **looking at apple**. X  
The **boy** is **looking at girl**. ✓



文本视觉生成

A **family** is **sitting at the table**, and  
there are **apples, bananas, and grapes** in the **bowl** on the table.

视觉问答

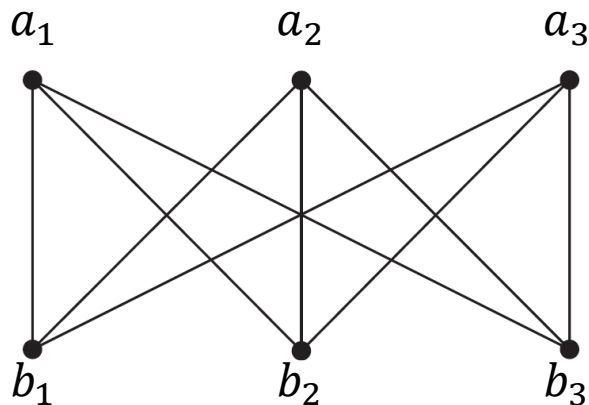
Q: Does **the boy** eat **bananas**?  
A: No.  
Q: What **fruit** is in the **bowl**?  
A: **Apple/Banana**

多模态模型

# Graph

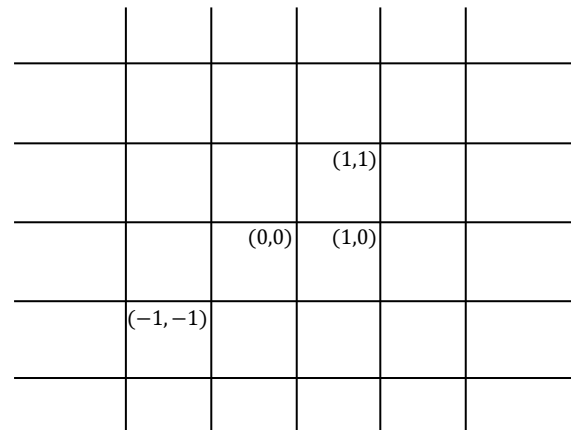
**DEFINITION:** A **graph**  $G = (V, E)$  is defined by a nonempty set  $V$  of **vertices**<sub>顶点</sub> and a set  $E$  of **edges**<sub>边</sub>, where each edge is associated with one or two vertices (called **endpoints**<sub>端点</sub> of the edge).

- **Infinite Graph**<sub>无限图</sub>:  $|V| = \infty$  or  $|E| = \infty$
- **Finite Graph**<sub>有限图</sub>:  $|V| < \infty$  and  $|E| < \infty$ ;  $|V|$  is called the **order**<sub>阶数</sub> of  $G$



$$V = \{a_1, a_2, a_3, b_1, b_2, b_3\}$$

$$E = \{\{a_i, b_j\} : i, j = 1, 2, 3\}$$



$$V = \{(i, j) : i, j \in \mathbb{Z}\}$$

$$E = \{\{(a, b), (c, d)\} : |a - c| = 1 \text{ or } |b - d| = 1\}$$

# Graphs

- Loop & multiple edge

An edge with one endpoint is called a **loop**.

If there is more than one edge between two distinct vertices, it is called a **multiple edge**.

- Simple graph

A **simple graph** is a finite graph with no loops nor multiple edges.

- Weighted graph

A **weighted graph** is a graph  $G = (V, E)$  such that each edge is assigned with a strictly positive number.



# Graphs

- Directed graph

A **directed graph**  $G = (V, E)$  consists of:

- $V$  a non empty set of **vertices**,
- $E$  a set of **directed edges**

Each edge  $e$  is associated with an **ordered pair of vertices**  $(u, v)$ , we say that  $e$  **starts at**  $u$  and **ends at**  $v$ .

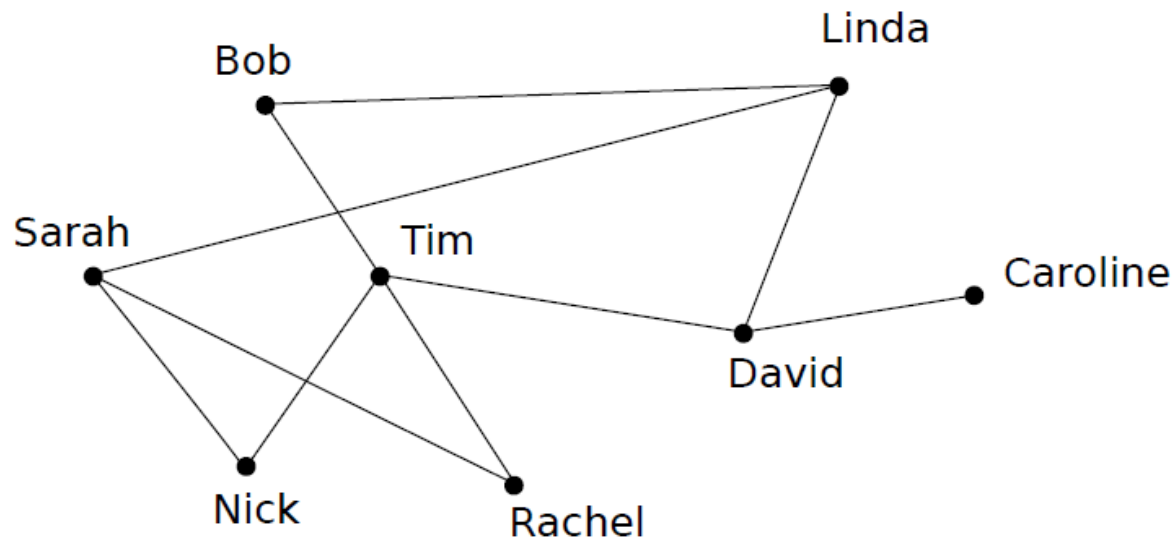
- Subgraph

A **subgraph** of a graph  $G = (V, E)$  is a graph  $H = (W, F)$  where  $W \subset V$ ,  $F \subset E$ . A subgraph  $H$  of  $G$  is a **proper subgraph** if  $H \neq G$ .



# Graph Examples

## Acquaintanceship Graph:



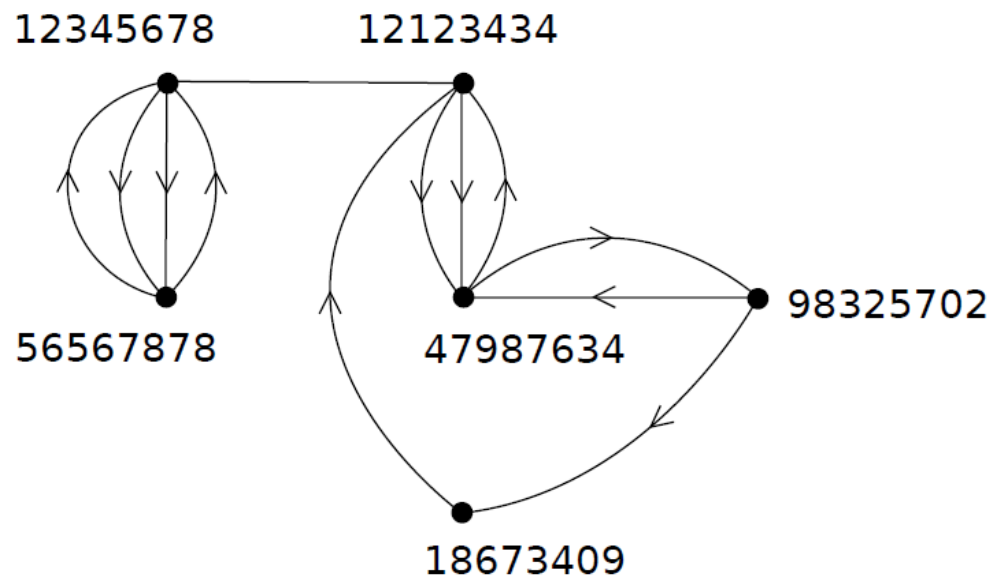
Tim knows Bob, David, Rachel and Nick. But Tim doesn't know Linda neither Caroline.

**Simple graph, undirected**

# Graph Examples

**Call Graphs:** directed edges; the same edge may appear multiple times

- Vertices: telephone numbers
- Edges: there is an arc  $(u, v)$  if  $u$  called  $v$
- AT&T experiment: calls during 20 days (290 million vertices and 4 billion edges)



Directed graph, multiple edges

# Graph Examples

## Precedence Graph

$S_1$   $a := 0$

$S_2$   $b := 1$

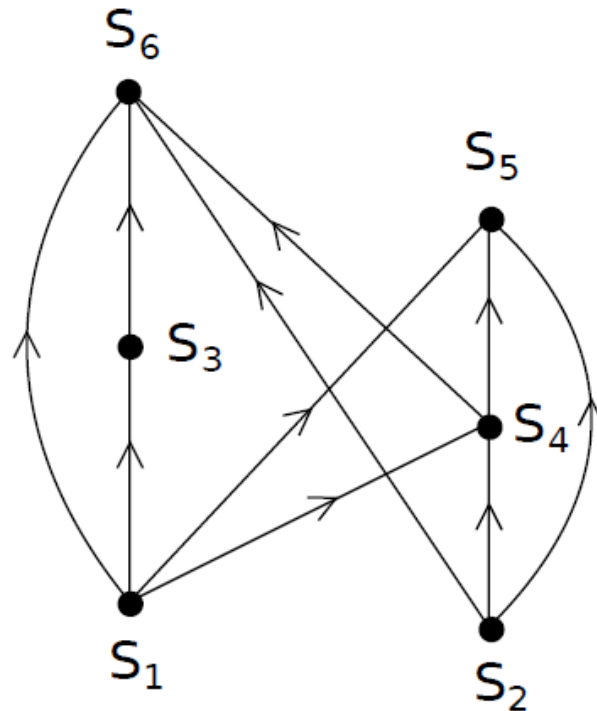
$S_3$   $c := a + 1$

$S_4$   $d := b + a$

$S_5$   $e := d + 1$

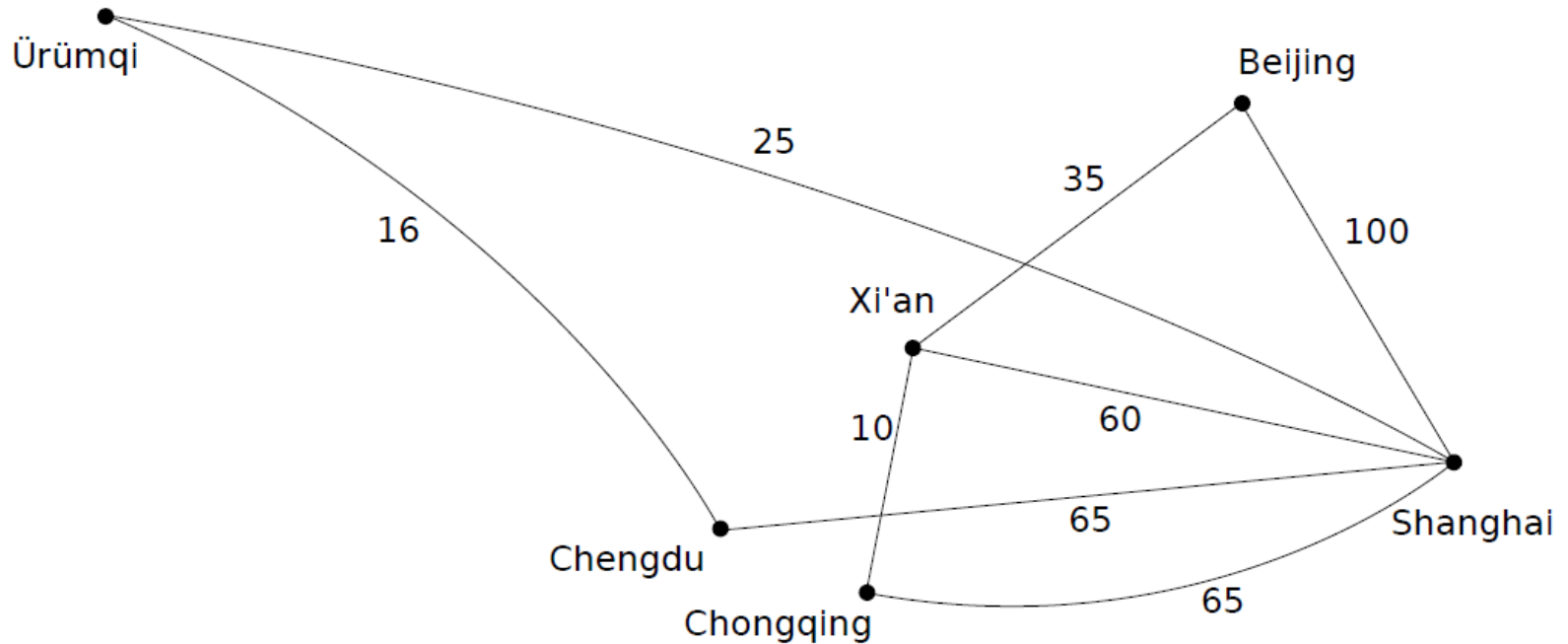
$S_6$   $f := c + d$

Directed simple graph



# Graph Examples

## Flights



## Weighted graph

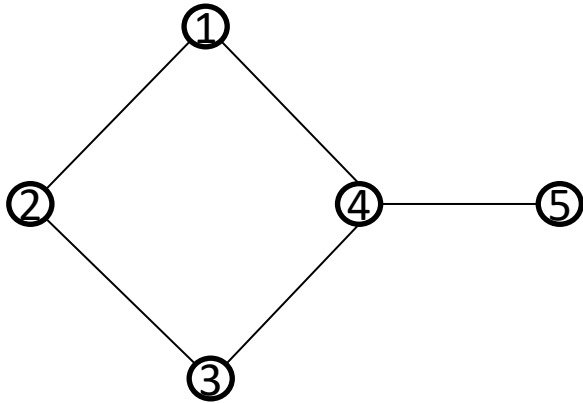
# Types of Graphs

**DEFINITION:** Let  $G = (V, E)$  be a graph with vertex set  $V = \{v_1, \dots, v_n\}$ .

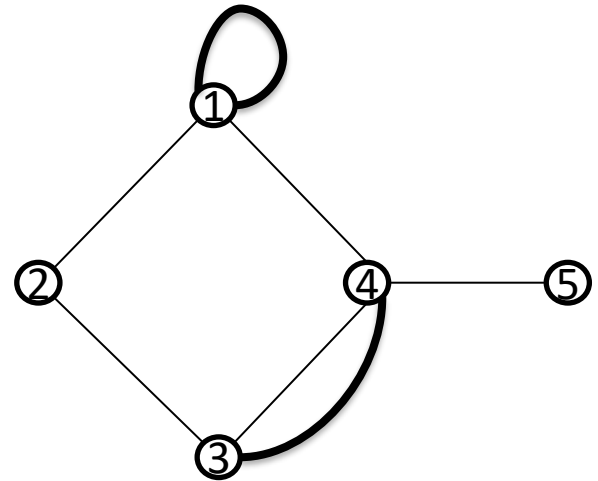
- **Question 1:** are the edges of  $G$  **directed**有向的?
  - No:  $G$  is an **undirected graph**无向图; the edge connecting  $v_i, v_j$ :  $\{v_i, v_j\}$
  - Yes:  $G$  is a **directed graph**有向图; the edge starting at  $v_i$  and ending at  $v_j$ :  $(v_i, v_j)$
- **Question 2:** are there **multiple edges**多重边 connecting two different vertices  $v_i, v_j$ ?
  - No:  $G$  is a **simple graph**简单图; Yes:  $G$  is a **multigraph**多重图
- **Question 3:** are there **loops**自环 connecting a vertex  $v_i$  to itself?
  - Yes:  $G$  is a **pseudograph**伪图

Type	Edges	Multiple Edges Allowed?	Loops Allowed?
Simple graph	undirected	No	No
Multigraph	undirected	Yes	No
Pseudograph	undirected	Yes	Yes
Simple directed graph	directed	No	No
Directed multigraph	directed	Yes	Yes
Mixed graph	undirected + directed	Yes	Yes

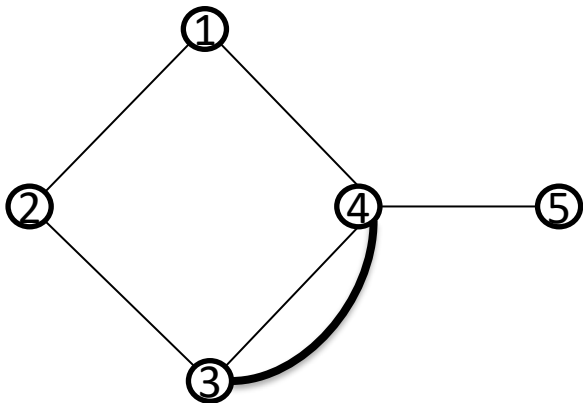
# Types of Graphs



A Simple Graph ( $G_1$ )



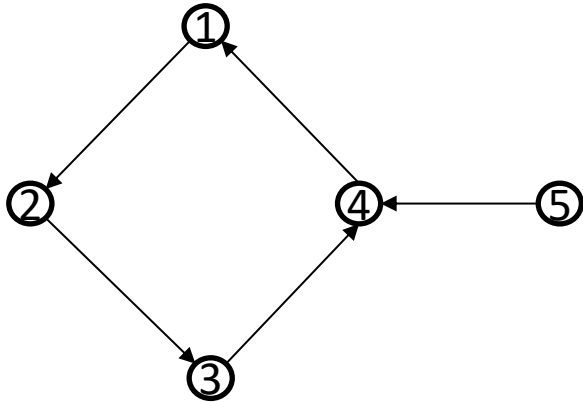
A Pseudograph ( $G_3$ )



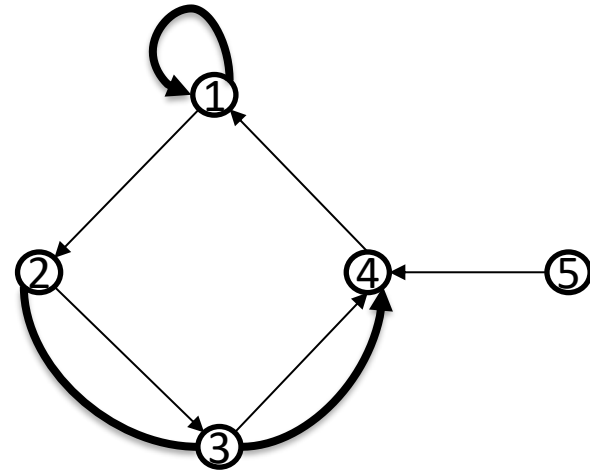
A Multigraph ( $G_2$ )

- Vertex set:  $V = \{1,2,3,4,5\}$
- Edge set of  $G_1$ :  $E = \{\{1,2\}, \{2,3\}, \{3,4\}, \{1,4\}, \{4,5\}\}$
- $\{4,5\}$  is an edge of the simple graph  $G_1$ 
  - 4,5 are endpoints of the edge  $\{4,5\}$
  - $\{4,5\}$  connects 4 and 5.
- $\{3,4\}$  is a multiple edge of the multigraph  $G_2$
- There is a loop connecting 1 to itself in  $G_3$

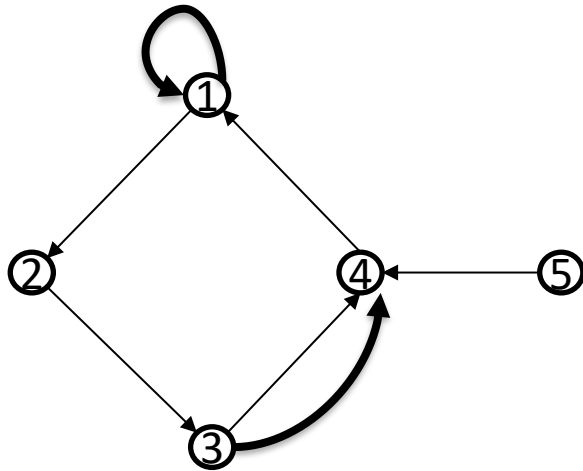
# Types of Graphs



A Simple Directed Graph ( $G_4$ )



A Mixed Graph ( $G_6$ )

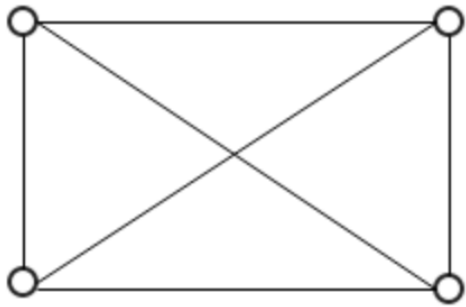


A Directed Multigraph ( $G_5$ )

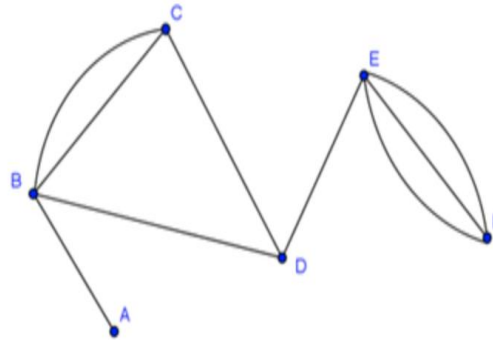
- Vertex set:  $V = \{1,2,3,4,5\}$
- Edge set of  $G_4$ :  $E = \{(1,2), (2,3), (3,4), (4,1), (5,4)\}$ 
  - $(5,4)$  is a directed edge
  - $(5,4)$  starts at 5 and ends at 4
- $(3,4)$  is a directed multiple edge in  $G_5$
- There is a loop connecting 1 to itself in  $G_5$



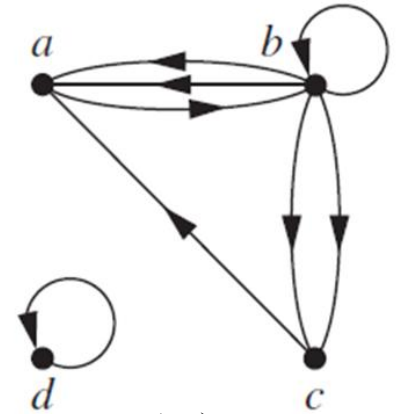
# Bonus exercise



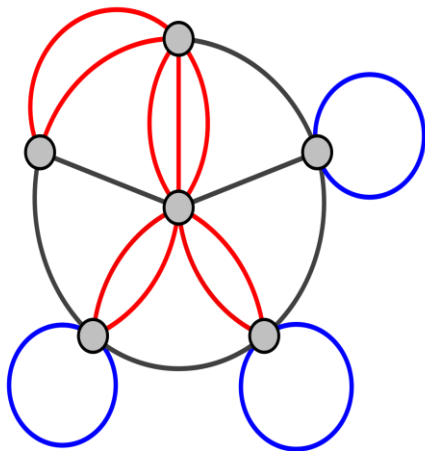
(1)



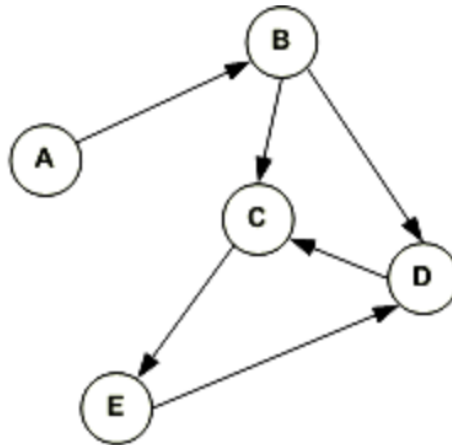
(3)



(5)

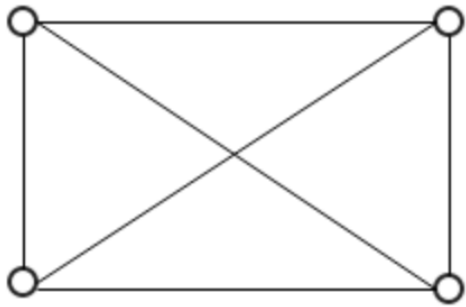


(2)

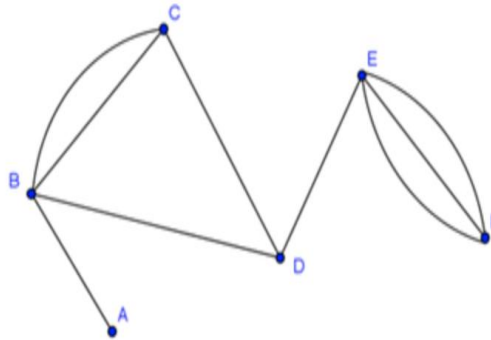


(4)

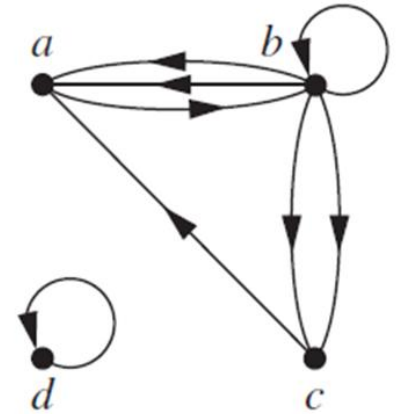
# Bonus exercise



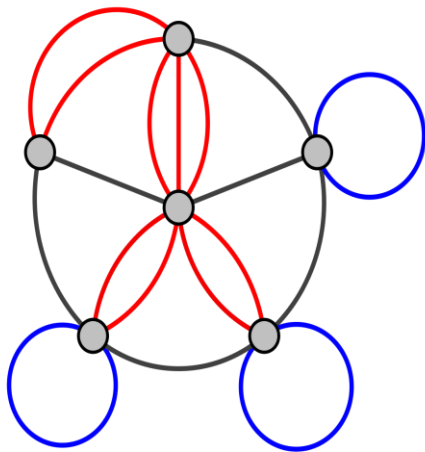
(1) simple graph



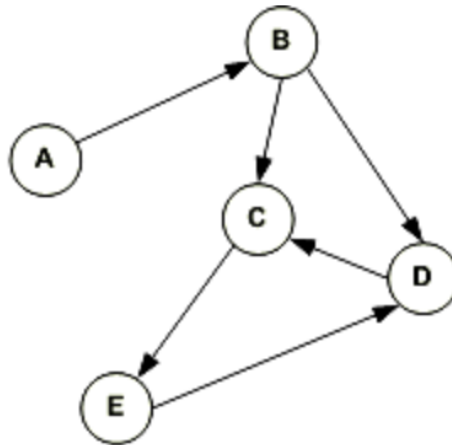
(3) multigraph



(5) directed multigraph



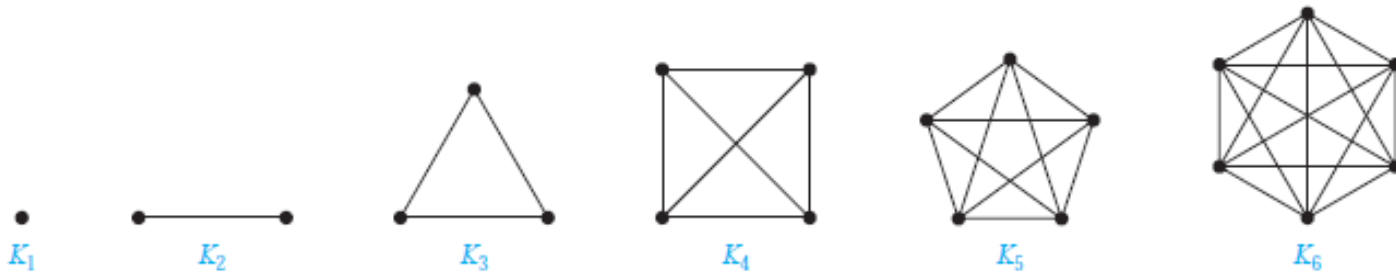
(2) pseudograph



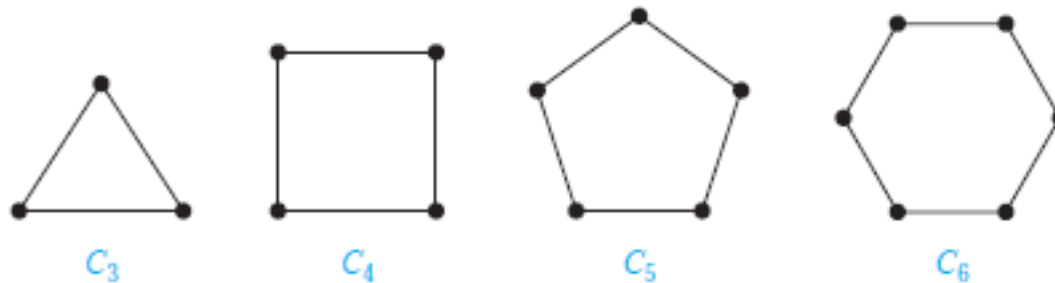
(4) simple directed graph

# Special Simple Graphs

**Complete Graph** 完全图  $K_n$ :  $V = \{v_1, \dots, v_n\}$ ;  $E = \{\{v_i, v_j\} : 1 \leq i \neq j \leq n\}$

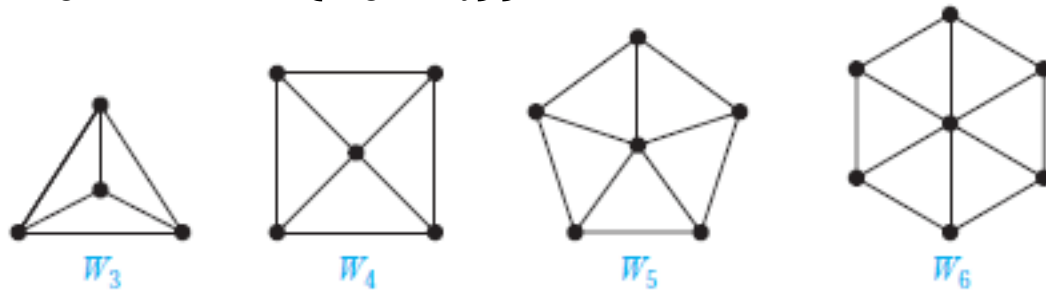


**Cycle** 环, 圈  $C_n$ :  $V = \{v_1, v_2, \dots, v_n\}$ ;  $E = \{\{v_1 v_2\}, \{v_2, v_3\}, \dots, \{v_n, v_1\}\}$



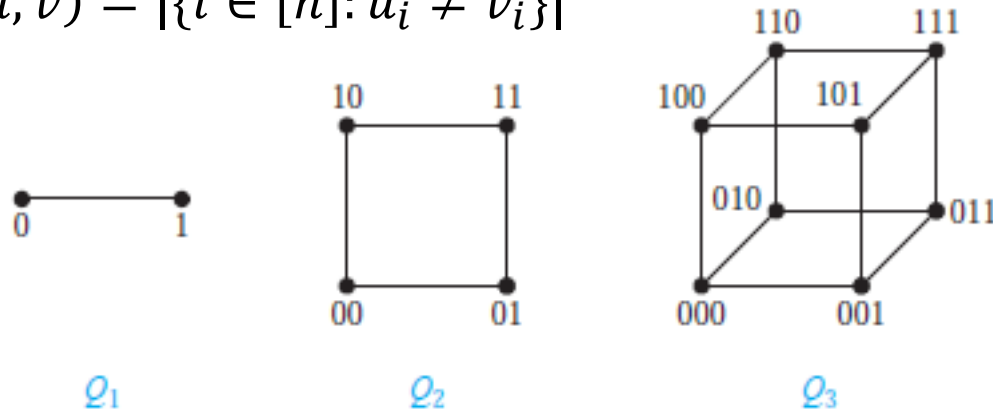
# Special Simple Graphs

**Wheel**<sub>轮</sub>  $W_n$ :  $V = \{v_0, v_1, v_2, \dots, v_n\}$ ;  $E = \{\{v_1, v_2\}, \dots, \{v_n, v_1\}\} \cup \{\{v_0, v_1\}, \dots, \{v_0, v_n\}\}$



**$n$ -Cubes**<sub>方体</sub>  $Q_n$ :  $V = \{0,1\}^n$ ;  $E = \{\{u, v\} : d(u, v) = 1\}$

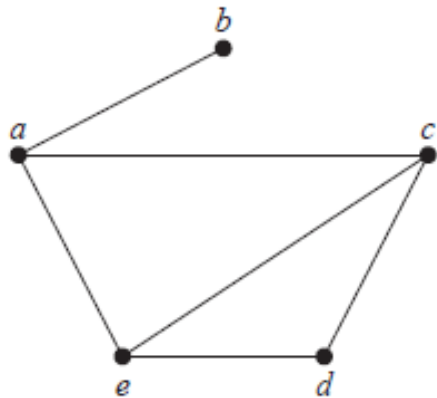
- $d(u, v) = |\{i \in [n] : u_i \neq v_i\}|$



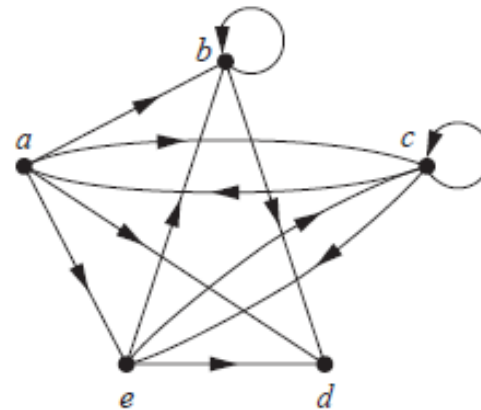
# Adjacency List

**DEFINITION:** Let  $G = (V, E)$  be a graph with no multiple edges. The **adjacency list**<sub>邻接表</sub> of  $G$  is a list the vertices of the graph and all adjacent vertices

- $v_i, v_j \in V$  are **adjacent**<sub>相邻的</sub> if  $\{v_i, v_j\}$  or  $(v_i, v_j)$  is an edge



$a$	$b, c, e$
$b$	$a$
$c$	$a, d, e$
$d$	$c, e$
$e$	$a, c, d$

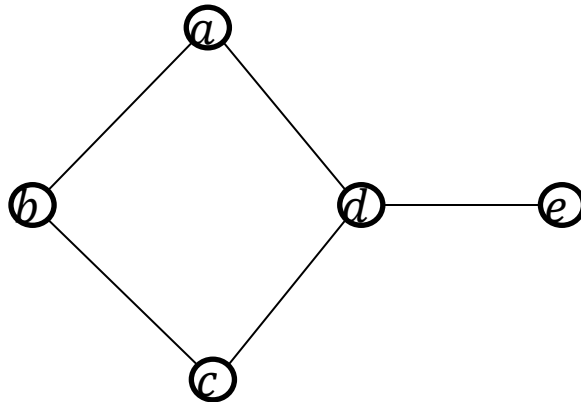


$a$	$b, c, d, e$
$b$	$b, d$
$c$	$a, c, e$
$d$	
$e$	$b, c, d$

# Adjacency Matrix

**DEFINITION:** Let  $G = (V = \{v_1, \dots, v_n\}, E)$  be a simple graph. The **adjacency matrix** 邻接矩阵 of  $G$  is an  $n \times n$  matrix  $A = (a_{ij})$ , where

$$a_{ij} = \begin{cases} 1 & \{v_i, v_j\} \in E \\ 0 & \{v_i, v_j\} \notin E \end{cases}$$

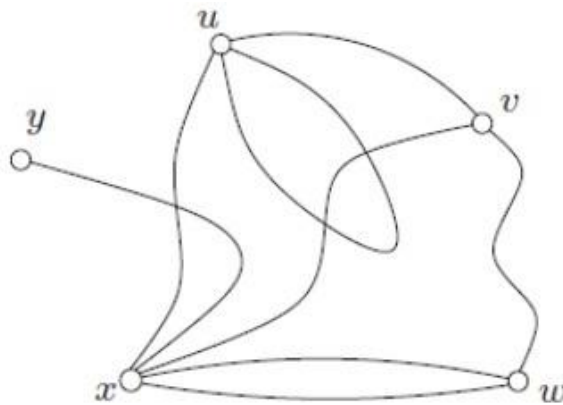


	$a$	$b$	$c$	$d$	$e$
$a$	0	1	0	1	0
$b$	1	0	1	0	0
$c$	0	1	0	1	0
$d$	1	0	1	0	1
$e$	0	0	0	1	0

# Adjacency Matrix

**DEFINITION:** Let  $G = (V = \{v_1, \dots, v_n\}, E)$  be an undirected graph. The **adjacency matrix** of  $G$  is an  $n \times n$  matrix  $A = (a_{ij})$ , where

- $a_{ij} = \text{multiplicity}_{\text{重数}}$  of  $\{v_i, v_j\}$  when  $i \neq j$
- $a_{ii} = 1$  if  $\exists$  a loop from  $v_i$  to itself;  $a_{ii} = 0$ , otherwise.



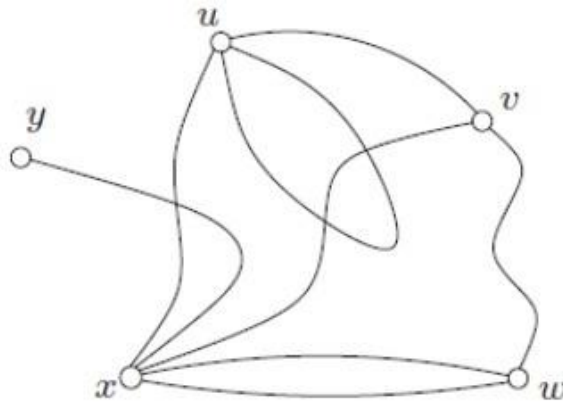
	$u$	$v$	$w$	$x$	$y$
$u$	1	1	0	1	0
$v$	1	0	1	1	0
$w$	0	1	0	2	0
$x$	1	1	2	0	1
$y$	0	0	0	1	0



# Adjacency Matrix

**DEFINITION:** Let  $G = (V = \{v_1, \dots, v_n\}, E)$  be an undirected graph. The **adjacency matrix** of  $G$  is an  $n \times n$  matrix  $A = (a_{ij})$ , where

- $a_{ij} = \text{multiplicity}_{\text{重数}}$  of  $\{v_i, v_j\}$  when  $i \neq j$
- $a_{ii} = 1$  if  $\exists$  a loop from  $v_i$  to itself;  $a_{ii} = 0$ , otherwise.



	$x$	$y$	$u$	$v$	$w$
$x$	0	1	1	1	2
$y$	1	0	0	0	0
$u$	1	0	1	1	0
$v$	1	0	1	0	1
$w$	2	0	0	1	0

**REMARKS:** features of the adjacency matrices of undirected graphs

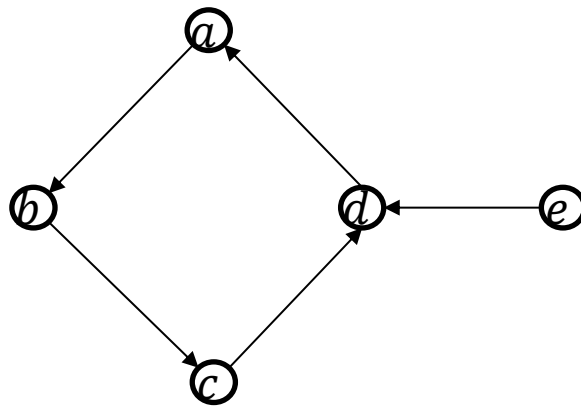
- The adjacency matrix depends on the ordering of the vertices
- The adjacency matrix of a simple graph is always symmetric
- The  $(i, j)$  entry counts the multiplicity of  $\{v_i, v_j\}$ ,  $i \neq j$

# Adjacency Matrix

**DEFINITION:** Let  $G = (V = \{v_1, \dots, v_n\}, E)$  be a simple directed graph.

The **adjacency matrix** of  $G$  is an  $n \times n$  matrix  $A = (a_{ij})$ , where

$$a_{ij} = \begin{cases} 1 & (v_i, v_j) \in E \\ 0 & (v_i, v_j) \notin E \end{cases}$$



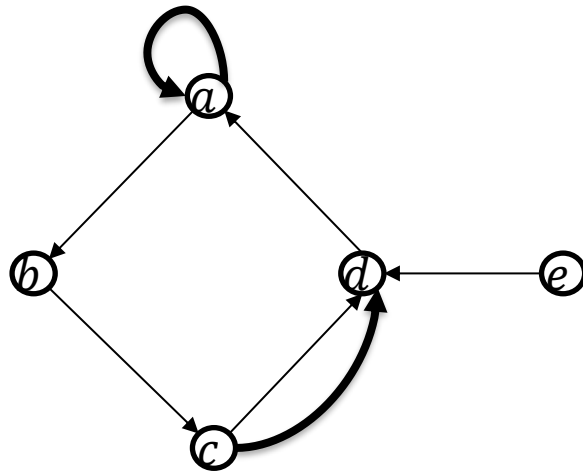
	<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>	<i>e</i>
<i>a</i>	0	1	0	0	0
<i>b</i>	0	0	1	0	0
<i>c</i>	0	0	0	1	0
<i>d</i>	1	0	0	0	0
<i>e</i>	0	0	0	1	0

**REMARKS:** The adjacency matrix is no longer symmetric

# Adjacency Matrix

**DEFINITION:** Let  $G = (V = \{v_1, \dots, v_n\}, E)$  be a directed multigraph. The **adjacency matrix** of  $G$  is an  $n \times n$  matrix  $A = (a_{ij})$ , where

$$a_{ij} = \begin{cases} \text{multiplicity of } (v_i, v_j) & (v_i, v_j) \in E \\ 0 & (v_i, v_j) \notin E \end{cases}$$



	$a$	$b$	$c$	$d$	$e$
$a$	1	1	0	0	0
$b$	0	0	1	0	0
$c$	0	0	0	2	0
$d$	1	0	0	0	0
$e$	0	0	0	1	0

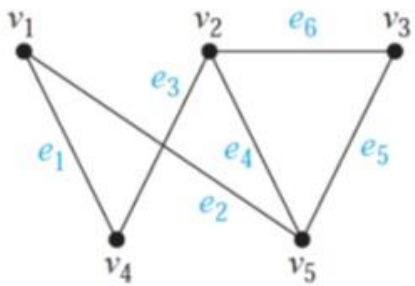
# Incidence Matrix

**DEFINITION:** Let  $G = (V = \{v_1, \dots, v_n\}, E = \{e_1, \dots, e_m\})$  be undirected.

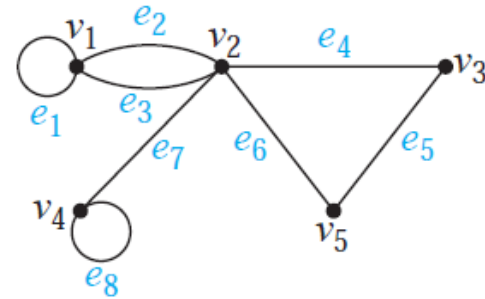
The **incidence matrix** 关联矩阵 of  $G$  is an  $n \times m$  matrix  $B = (b_{ij})$ , where

$$b_{ij} = \begin{cases} 1 & \text{if } e_j \text{ is incident with } v_i \\ 0 & \text{otherwise} \end{cases}$$

- $e_j$  **incident with**  $v_i$ :  $v_i$  is an endpoint of  $e_j$



$$\begin{matrix} & e_1 & e_2 & e_3 & e_4 & e_5 & e_6 \\ \begin{matrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \end{matrix} & \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 \end{bmatrix} \end{matrix}$$

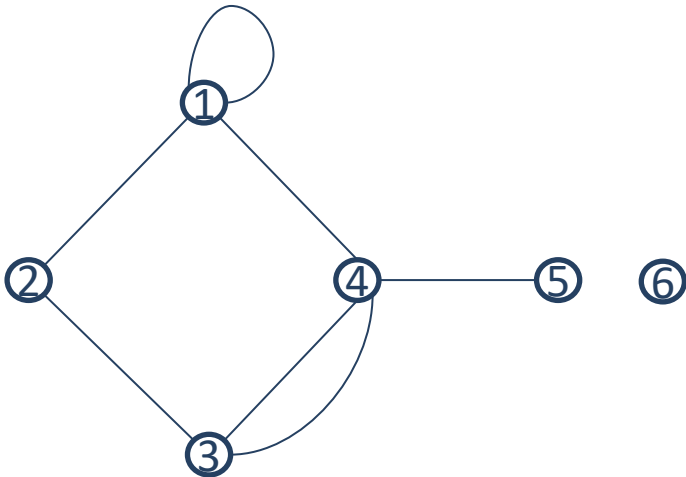


$$\begin{matrix} & e_1 & e_2 & e_3 & e_4 & e_5 & e_6 & e_7 & e_8 \\ \begin{matrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \end{matrix} & \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{bmatrix} \end{matrix}$$

# Degree

**DEFINITION:** Let  $G = (V, E)$  be an undirected graph. We say that two vertices  $u, v \in V$  are **adjacent**<sub>相邻的</sub> (or **neighbors**<sub>邻居</sub>) if  $\{u, v\} \in E$ .

- **neighborhood**<sub>邻域</sub> of  $v$  in  $G$ :  $N(v) = \{u \in V : \{u, v\} \in E\}$ 
  - $N(A) = \bigcup_{v \in A} N(v)$  for  $A \subseteq V$
- the **degree**<sub>度</sub>  $\deg(v)$  of  $v \in V$  in  $G$ , is the number of edges incident with  $v$ 
  - every loop from  $v$  to  $v$  contributes 2 to  $\deg(v)$
- $v$  is **isolated**<sub>孤立的</sub> if  $\deg(v) = 0$ ;  $v$  is **pendant**<sub>悬挂的</sub> if  $\deg(v) = 1$

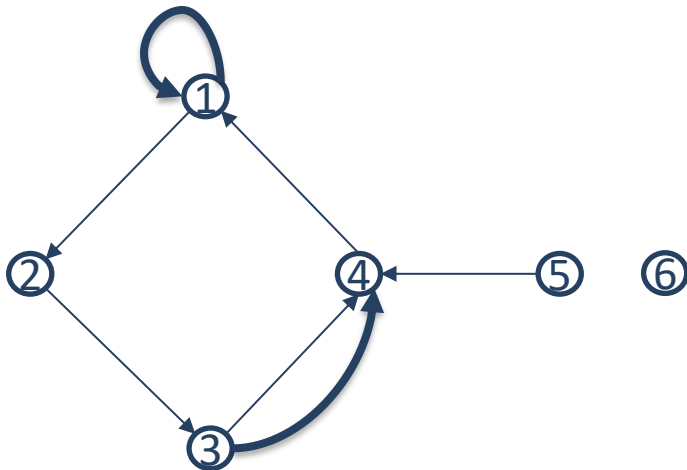


- 4 and 5 are adjacent
- $\{4, 5\}$  is incident with 4 and 5
- $N(4) = \{1, 3, 5\}$ ;  $N(\{1, 4\}) = \{1, 2, 3, 4, 5\}$
- $\deg(1) = 4$ ,  $\deg(2) = 2$ ,  $\deg(3) = 3$ ,  $\deg(4) = 4$ ,  $\deg(5) = 1$
- 6 is isolated; 5 is pendant

# Degree

**DEFINITION:** Let  $G = (V, E)$  be a directed graph. If  $(u, v) \in E$ , we say that  $u$  is **adjacent to**  $v$  and  $v$  is **adjacent from**  $u$ .

- $u$  is the **initial vertex**<sub>起始点</sub> of  $(u, v)$ ;  $v$  is the **terminal vertex**<sub>终点</sub> of  $(u, v)$ 
  - $u = v$ :  $u$  is the initial vertex and the terminal vertex
- **in-degree**<sub>入度</sub>  $\deg^-(v)$ : the number of edges where  $v$  is the terminal vertex
- **out-degree**<sub>出度</sub>  $\deg^+(v)$ : the number of edges where  $v$  is the initial vertex
  - $u = v$ : the loop contributes 1 to  $\deg^-(v)$  and 1 to  $\deg^+(v)$



- 5 is adjacent to 4; 4 is adjacent from 5
- 5 is the initial vertex of  $(5, 4)$
- 4 is the terminal vertex of  $(5, 4)$
- 1 is the initial and terminal vertex of a loop
- $\deg^-(1) = 2$ ;  $\deg^+(1) = 2$
- $\deg^-(4) = 3$ ;  $\deg^+(4) = 1$

# Handshaking Theorem

**THEOREM:** Let  $G = (V, E)$  be an undirected graph. Then

$2|E| = \sum_{v \in V} \deg(v)$  and  $|\{v \in V : \deg(v) \text{ is odd}\}|$  is even.

- Any edge  $e \in E$  contribute 2 to the sum  $\sum_{v \in V} \deg(v)$ 
  - $e = \{v_i, v_j\}$ :  $e$  contributes 1 to  $\deg(v_i)$  and 1 to  $\deg(v_j)$
  - $e = \{v_i\}$ :  $e$  contributes 2 to  $\deg(v_i)$
- The  $m$  edges contribute  $2|E|$  to  $\sum_{v \in V} \deg(v)$ .
  - Hence,  $\sum_{v \in V} \deg(v) = 2|E|$
- $\sum_{v \in V} \deg(v) = \sum_{v \in V: 2 \mid \deg(v)} \deg(v) + \sum_{v \in V: 2 \nmid \deg(v)} \deg(v)$ 
  - $2 \mid \sum_{v \in V} \deg(v)$ ;  $2 \mid \sum_{v \in V: 2 \mid \deg(v)} \deg(v)$ 
    - $2 \mid \sum_{v \in V: 2 \nmid \deg(v)} \deg(v)$ 
      - $|\{v \in V : \deg(v) \text{ is odd}\}|$  must be even

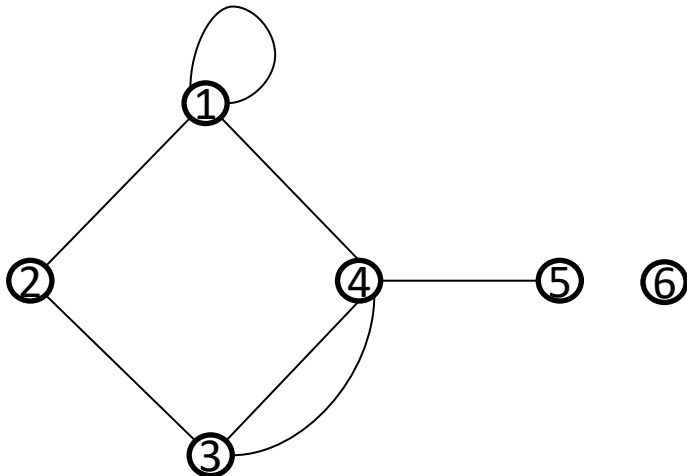


# Handshaking Theorem

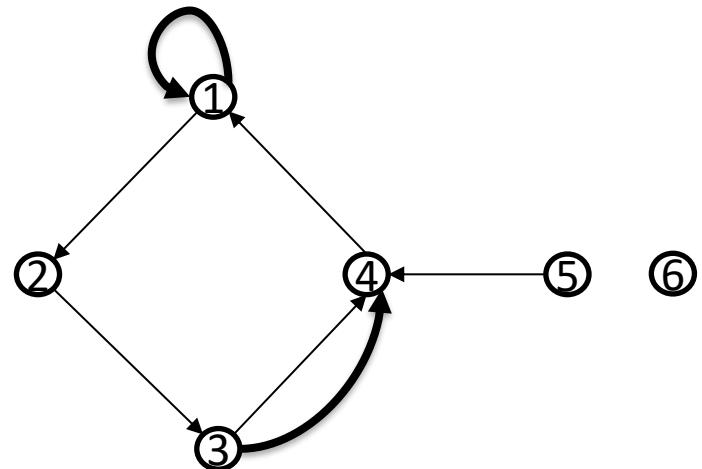
**THEOREM:** Let  $G = (V, E)$  be a directed graph. Then

$$\sum_{v \in V} \deg^-(v) = \sum_{v \in V} \deg^+(v) = |E|.$$

- Every edge  $e \in E$  contributes 1 to  $\sum_{v \in V} \deg^-(v)$ 
  - $e = (v_i, v_j)$  contributes 1 to  $\deg^-(v_i)$
- Hence,  $\sum_{v \in V} \deg^-(v) = |E|$



$v$	1	2	3	4	5	6
$\deg(v)$	4	2	3	4	1	0



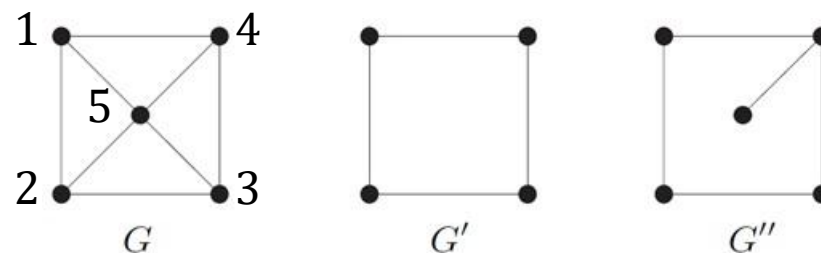
$v$	1	2	3	4	5	6
$\deg^-(v)$	2	1	1	3	0	0
$\deg^+(v)$	2	1	2	1	1	0

# Subgraph

**DEFINITION:** Let  $G = (V, E)$  be a simple graph.  $H = (W, F)$  is a **subgraph**<sub>子图</sub> of  $G$  if  $W \subseteq V$  and  $F \subseteq E$ .

- **proper subgraph**<sub>真子图</sub>:  $H$  is a subgraph of  $G$  and  $H \neq G$ .
- The **subgraph induced**<sub>导出子图</sub> by  $W \subseteq V$  is  $(W, F)$ , where  $F = \{e: e \in E, e = \{u, v\} \subseteq W\}$ . //Notation:  $G[W]$
- The **subgraph induced**<sub>导出子图</sub> by  $F \subseteq E$  is  $(W, F)$ , where  $W = \{v: v \in V, v \in e \text{ for some } e \in F\}$ . //Notation:  $G[F]$

**EXAMPLE:** Let  $G, G', G''$  be three graphs as below.

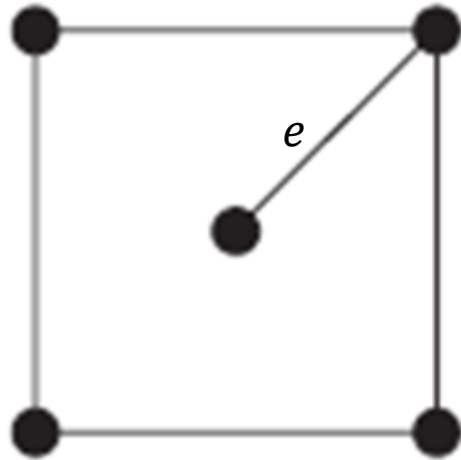


- $G', G''$  are subgraphs of  $G$ ;  $G', G''$  are proper subgraphs of  $G$
- $G'$  is a subgraph induced by  $W = \{1, 2, 3, 4\}$ , i.e.,  $G' = G[W]$
- $G''$  is a subgraph induced by  $F = \{\{1, 2\}, \{2, 3\}, \{3, 4\}, \{4, 1\}, \{4, 5\}\}$ , i.e.,  $G'' = G[F]$

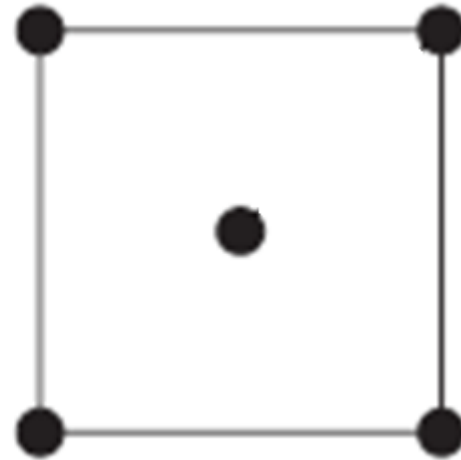
# Removing An Edge

**DEFINITION:** Let  $G = (V, E)$  be a simple graph and  $e \in E$ . Define

$$G - e = (V, E - \{e\})$$



$$G = (V, E)$$

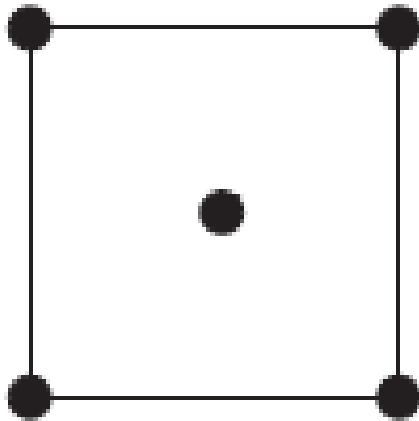


$$G - e = (V, E - \{e\})$$

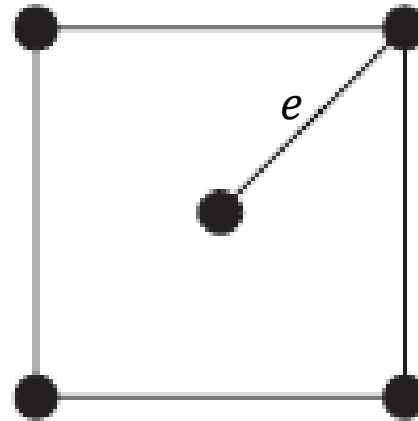
# Adding An Edge

**DEFINITION:** Let  $G = (V, E)$  be a simple graph and  $e \notin E$ . Define

$$G + e = (V, E \cup \{e\})$$



$$G = (V, E)$$



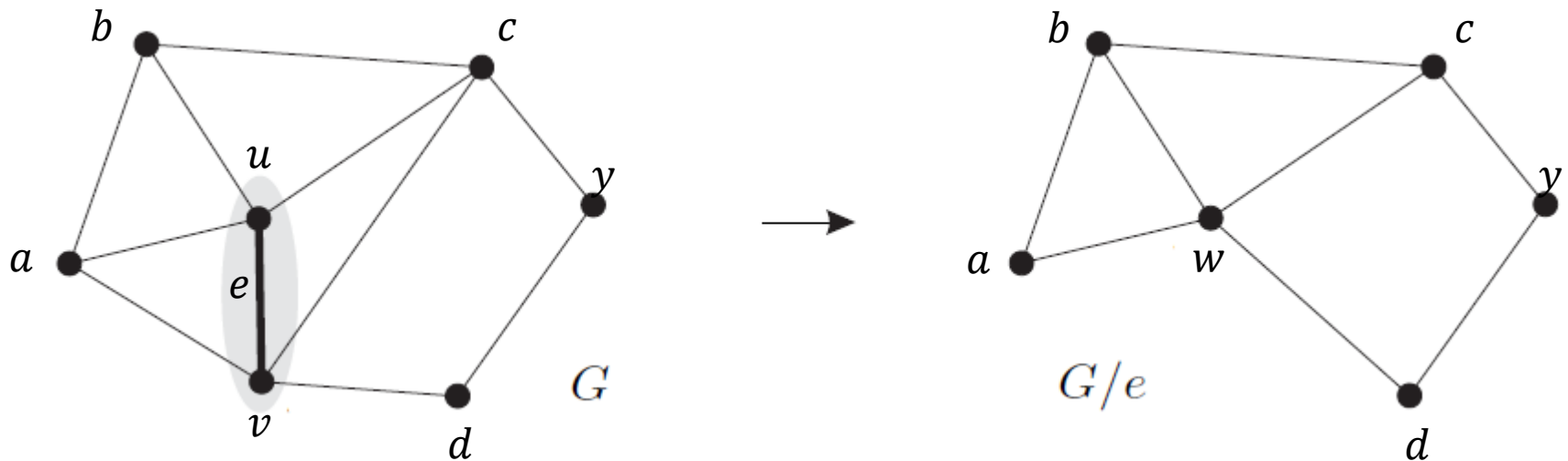
$$G + e = (V, E \cup \{e\})$$

# Edge Contraction

**DEFINITION:** Let  $G = (V, E)$  be a simple graph and  $e = \{u, v\} \in E$ .

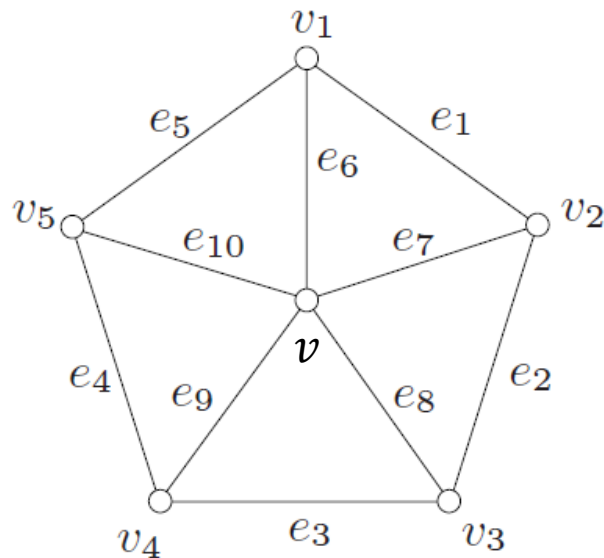
Define  $G/e = (V', E')$ , where  $V' = (V - \{u, v\}) \cup \{w\}$  and

$E' = \{e' \in E : e' \cap e = \emptyset\} \cup \{\{w, x\} : \{u, x\} \in E \text{ or } \{v, x\} \in E\}$

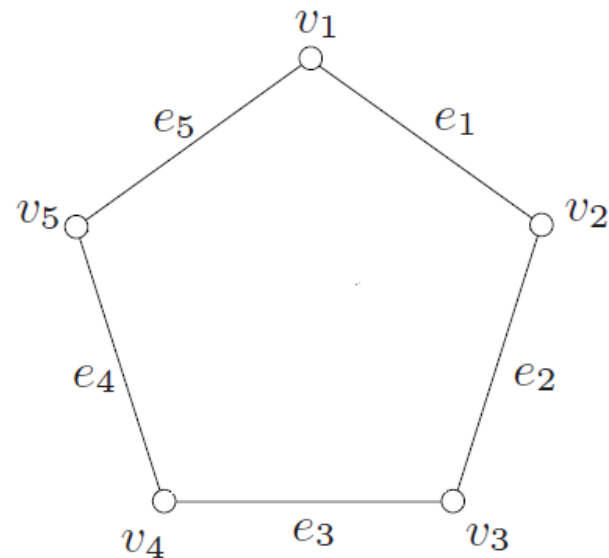


# Removing A Vertex

**DEFINITION:** Let  $G = (V, E)$  be a simple graph and let  $v \in V$ . Define  $G - v = (V - \{v\}, E')$ , where  $E' = \{e \in E : v \notin e\}$



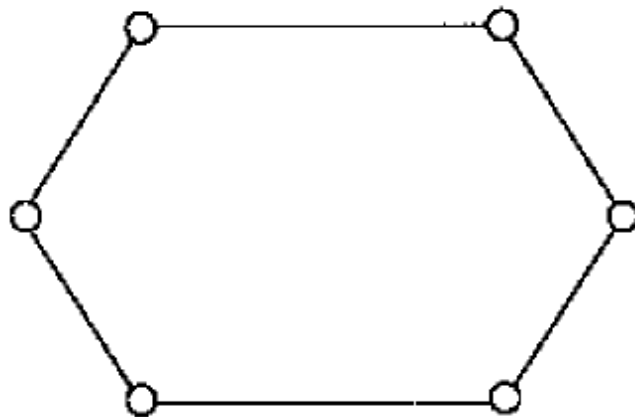
$G = (V, E)$



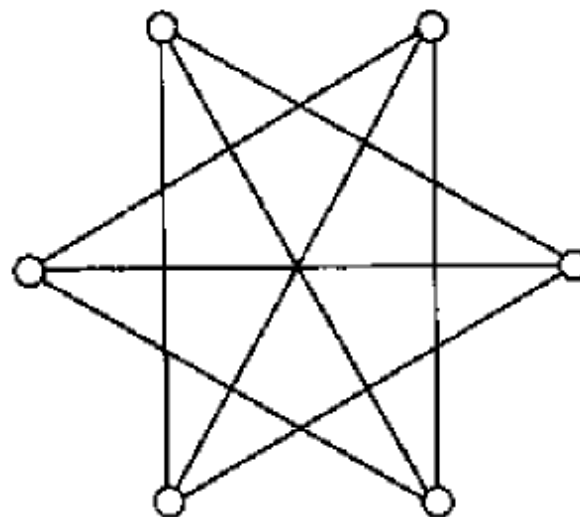
$G - v$

# Complement

**DEFINITION:** Let  $G = (V, E)$  be a simple graph of order  $n$ . Define the **complement graph** 补图 of  $G$  as  $\bar{G} = (V, E')$ , where

$$E' = \{\{u, v\} : u, v \in V, u \neq v, \{u, v\} \notin E\}$$


$G$



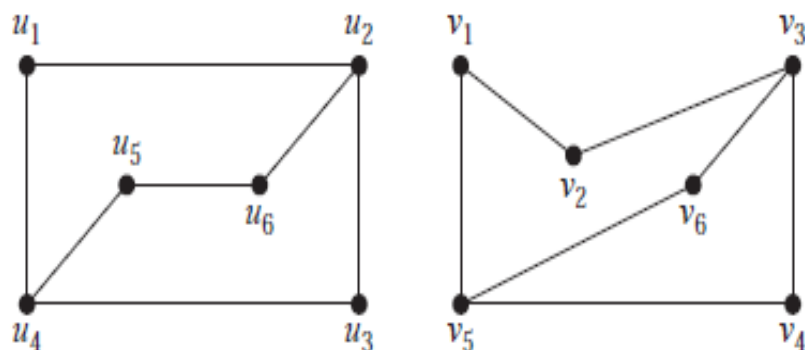
$\bar{G}$



# Graph Isomorphism

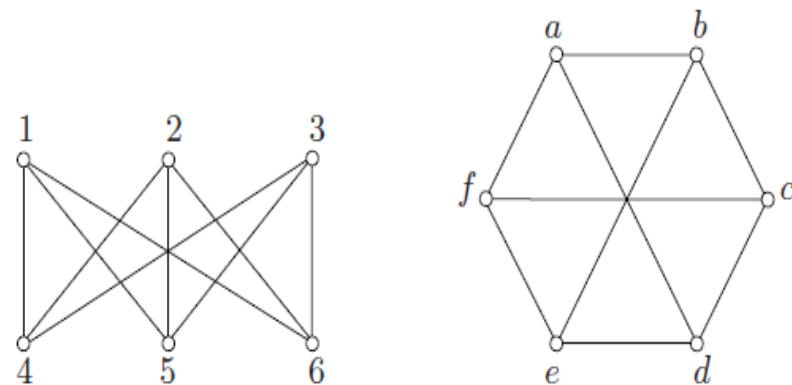
**DEFINITION:** The simple graphs  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  are **isomorphic** 同构 if there is a bijection  $\sigma: V_1 \rightarrow V_2$  such that  $\{u, v\} \in E_1 \Leftrightarrow \{\sigma(u), \sigma(v)\} \in E_2$ .

- $\sigma$  is called an **isomorphism** 同构映射
- nonisomorphic:** not isomorphic



$u_1$	$u_2$	$u_3$	$u_4$	$u_5$	$u_6$
$v_6$	$v_3$	$v_4$	$v_5$	$v_1$	$v_2$

Isomorphism  $\sigma$



1	2	3	4	5	6
$a$	$c$	$e$	$b$	$d$	$f$

Isomorphism  $\sigma$