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Mathematical Foundations for Data Science

MFDS Team

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DSECL ZC416, MFDS

Lecture No.14

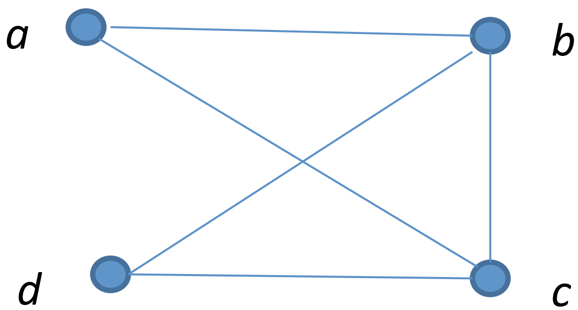
Agenda

- Graphs and Terminology
- Graph Models and Applications
- Hand Shaking Theorem
- Simple Graph and its types
- Bipartite Graphs
- Representation of graphs
  - Adjacency List
  - Incidence Matrices

Graphs

Definition: A *graph* $G = (V, E)$ consists of a nonempty set V of *vertices* (or *nodes*) and a set E of *edges*. Each edge has either one or two vertices associated with it, called its *endpoints*. An edge is said to *connect* its endpoints.

Example:



This is a graph with four vertices and five edges.

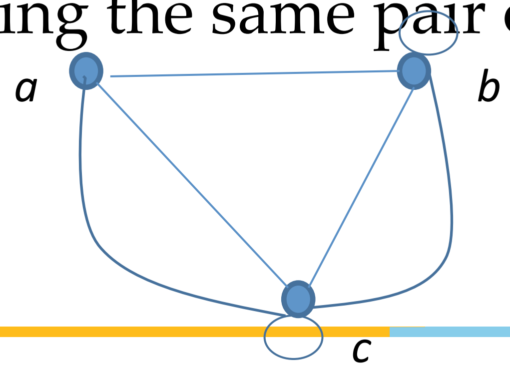
Remarks:

- The graphs we study here are unrelated to graphs of functions
- We have a lot of freedom when we draw a picture of a graph. All that matters is the connections made by the edges, not the particular geometry depicted. For example, the lengths of edges, whether edges cross, how vertices are depicted, and so on, do not matter
- A graph with an infinite vertex set is called an *infinite graph*. A graph with a finite vertex set is called a *finite graph*. We (following the text) restrict our attention to finite graphs.

Some Terminology

- In a *simple graph* each edge connects two different vertices and no two edges connect the same pair of vertices.
- *Multigraphs* may have multiple edges connecting the same two vertices. When m different edges connect the vertices u and v, we say that $\{u,v\}$ is an edge of *multiplicity* m.
- An edge that connects a vertex to itself is called a *loop*.
- A *pseudograph* may include loops, as well as multiple edges connecting the same pair of vertices.

Example:
This pseudograph has both multiple edges and a loop.



Remark: There is no standard terminology for graph theory. So, it is crucial that you understand the terminology being used whenever you read material about graphs.

Directed Graphs

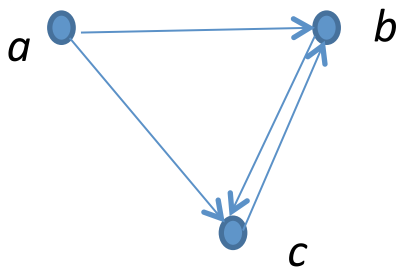
Definition: An *directed graph* (or *digraph*) $G = (V, E)$ consists of a nonempty set V of *vertices* (or *nodes*) and a set E of *directed edges* (or *arcs*). Each edge is associated with an ordered pair of vertices. The directed edge associated with the ordered pair (u,v) is said to *start at u* and *end at v*.

Remark:

- Graphs where the end points of an edge are not ordered are said to be *undirected graphs*.

Some Terminology (*continued*)

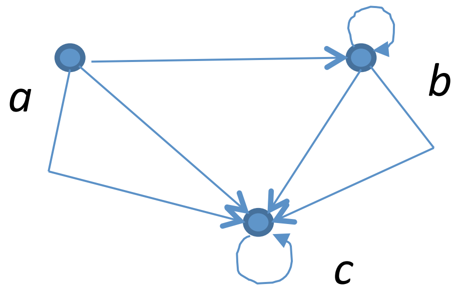
A *simple directed graph* has no loops and no multiple edges.



Example: This is a directed graph with three vertices and four edges.

A *directed multigraph* may have multiple directed edges. When there are m directed edges from the vertex u to the vertex v, we say that (u,v) is an edge of *multiplicity* m.

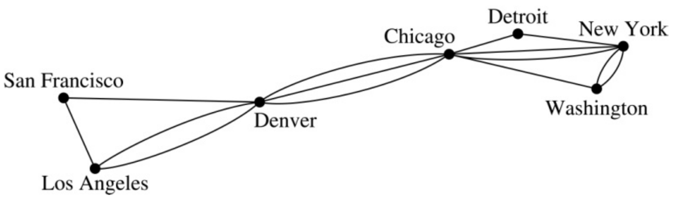
Example:



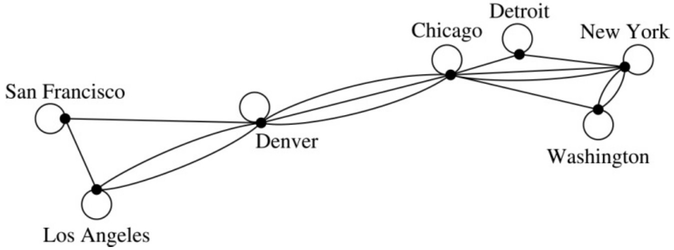
In this directed multigraph the multiplicity of (a,b) is 1 and the multiplicity of (b,c) is 2.

Graph Models: Computer Networks

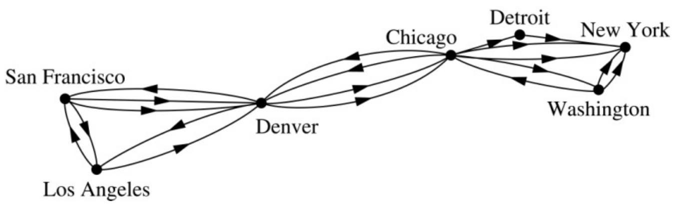
- To model a computer network where we care about the number of links between data centers, we use a multigraph.



- To model a computer network with diagnostic links at data centers, we use a pseudograph, as loops are needed.



- To model a network with multiple one-way links, we use a directed multigraph. Note that we could use a directed graph without multiple edges if we only care whether there is at least one link from a data center to another data center.



Graph Terminology: Summary

To understand the structure of a graph and to build a graph model, we ask these questions:

- Are the edges of the graph undirected or directed (or both)?
- If the edges are undirected, are multiple edges present that connect the same pair of vertices? If the edges are directed, are multiple directed edges present?
- Are loops present?

TABLE 1 **Graph Terminology.**

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	Directed and undirected	Yes	Yes

Other Applications of Graphs

We will illustrate how graph theory can be used in models of:

- Social networks
- Communications networks
- Information networks
- Software design
- Transportation networks
- Biological networks

It's a challenge to find a subject to which graph theory has not yet been applied.

Can you find an area without applications of graph theory?

Examples of Collaboration Graphs

An *academic collaboration graph* models the collaboration of researchers who have jointly written a paper in a particular subject.

- We represent researchers in a particular academic discipline using vertices.
- We connect the vertices representing two researchers in this discipline if they are coauthors of a paper.
- We will study the academic collaboration graph for mathematicians when we discuss *Erdős numbers* in Section 10.4.

Transportation Graphs

Graph models are extensively used in the study of transportation networks.

Airline networks can be modeled using directed multigraphs where

– airports are represented by vertices

– each flight is represented by a directed edge from the vertex representing the departure airport to the vertex representing the destination airport

Road networks can be modeled using graphs where

– vertices represent intersections and edges represent roads.

– undirected edges represent two-way roads and directed edges represent one-way roads.

Definition 1. Two vertices u, v in an undirected graph G are called *adjacent* (or *neighbors*) in G if there is an edge e between u and v. Such an edge e is called *incident with* the vertices u and v and e is said to *connect* u and v.

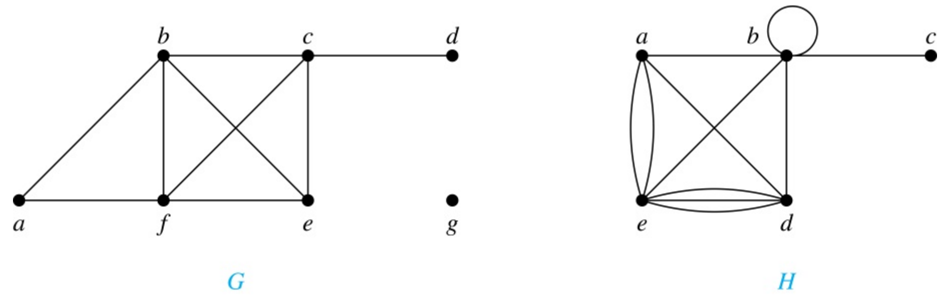
Definition 2. The set of all neighbors of a vertex v of $G = (V, E)$, denoted by $N(v)$, is called the *neighborhood* of v. If A is a subset of V, we denote by $N(A)$ the set of all vertices in G that are adjacent to at least one vertex in A. So,

$$N(A) = \bigcup_{v \in A} N(v).$$

Definition 3. The *degree of a vertex in a undirected graph* is the number of edges incident with it, except that a loop at a vertex contributes two to the degree of that vertex. The degree of the vertex v is denoted by $\deg(v)$.

Degrees and Neighborhoods of Vertices

Example: What are the degrees and neighborhoods of the vertices in the graphs G and H?



Solution:

G: $\deg(a) = 2$, $\deg(b) = \deg(c) = \deg(f\,) = 4$, $\deg(d\,) = 1$,
$\deg(e) = 3$, $\deg(g) = 0$.
$N(a) = \{b, f\,\}$, $N(b) = \{a, c, e, f\,\}$, $N(c) = \{b, d, e, f\,\}$, $N(d) = \{c\}$,
$N(e) = \{b, c\,, f\,\}$, $N(f) = \{a, b, c, e\}$, $N(g) = \varnothing$.

H: $\deg(a) = 4$, $\deg(b) = \deg(e) = 6$, $\deg(c) = 1$, $\deg(d) = 5$.
$N(a) = \{b, d, e\}$, $N(b) = \{a, b, c, d, e\}$, $N(c) = \{b\}$,
$N(d) = \{a, b, e\}$, $N(e) = \{a, b\,, d\}$.

Degrees of Vertices

Theorem 1 (*Handshaking Theorem*): If $G = (V,E)$ is an undirected graph with m edges, then

$$2m = \sum_{v \in V} \deg(v)$$

Proof:

Each edge contributes twice to the degree count of all vertices. Hence, both the left-hand and right-hand sides of this equation equal twice the number of edges.

Think about the graph where vertices represent the people at a party and an edge connects two people who have shaken hands.

Handshaking Theorem

We now give two examples illustrating the usefulness of the handshaking theorem.

Example: How many edges are there in a graph with 10 vertices of degree six?

Solution: Because the sum of the degrees of the vertices is $6 \cdot 10 = 60$, the handshaking theorem tells us that $2m = 60$. So the number of edges $m = 30$.

Example: If a graph has 5 vertices, can each vertex have degree 3?

Solution: This is not possible by the handshaking theorem, because the sum of the degrees of the vertices $3 \cdot 5 = 15$ is odd.

Degree of Vertices

Theorem 2: An undirected graph has an even number of vertices of odd degree.

Proof: Let V_1 be the vertices of even degree and V_2 be the vertices of odd degree in an undirected graph $G = (V, E)$ with m edges. Then

even $\rightarrow$ $$2m = \sum_{v \in V} \deg(v) = \sum_{v \in V_1} \deg(v) + \sum_{v \in V_2} \deg(v).$$

must be even since $\deg(v)$ is even for each $v \in V_1$

This sum must be even because $2m$ is even and the sum of the degrees of the vertices of even degrees is also even. Because this is the sum of the degrees of all vertices of odd degree in the graph, there must be an even number of such vertices.

Directed Graphs

Recall the definition of a directed graph.

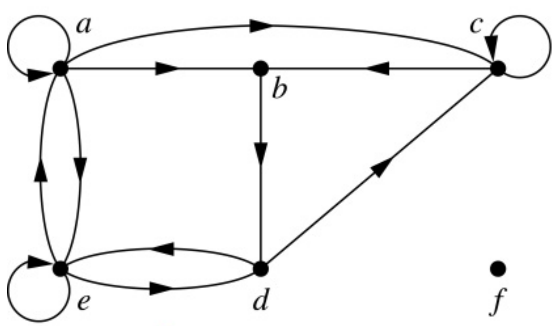
Definition: An *directed graph* $G = (V, E)$ consists of V, a nonempty set of *vertices* (or *nodes*), and E, a set of *directed edges* or *arcs*. Each edge is an ordered pair of vertices. The directed edge (u,v) is said to start at u and end at v.

Definition: Let (u,v) be an edge in G. Then u is the *initial vertex* of this edge and is *adjacent to* v and v is the *terminal* (or *end*) *vertex* of this edge and is *adjacent from* u. The initial and terminal vertices of a loop are the same.

Directed Graphs

Definition: The *in-degree of a vertex* v, denoted $deg^-(v)$, is the number of edges which terminate at v. The *out-degree of* v, denoted $deg^+(v)$, is the number of edges with v as their initial vertex. Note that a loop at a vertex contributes 1 to both the in-degree and the out-degree of the vertex.

Example: In the graph G we have



G

$deg^-(a) = 2$, $deg^-(b) = 2$, $deg^-(c) = 3$, $deg^-(d) = 2$,
$deg^-(e) = 3$, $deg^-(f) = 0$.

$deg^+(a) = 4$, $deg^+(b) = 1$, $deg^+(c) = 2$, $deg^+(d) = 2$,
$deg^+(e) = 3$, $deg^+(f) = 0$.

Directed Graphs

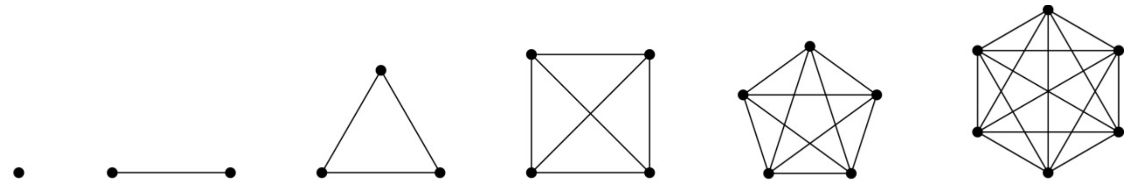
Theorem 3: Let $G = (V, E)$ be a graph with directed edges. Then:

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

Proof: The first sum counts the number of outgoing edges over all vertices and the second sum counts the number of incoming edges over all vertices. It follows that both sums equal the number of edges in the graph.

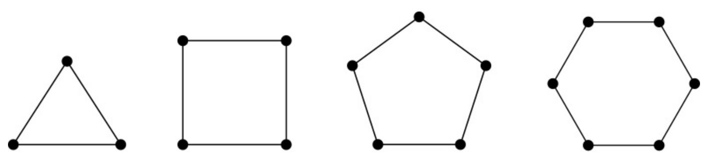
Special Types of Simple Graphs

A *complete graph on n vertices*, denoted by K_n, is the simple graph that contains exactly one edge between each pair of distinct vertices.



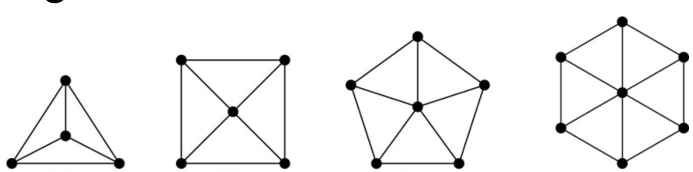
K_1 K_2 K_3 K_4 K_5 K_6

A *cycle* C_n for $n \geq 3$ consists of n vertices $v_1, v_2, \cdots, v_n$, and edges $\{v_1, v_2\}$, $\{v_2, v_3\}, \cdots, \{v_{n-1}, v_n\}$, $\{v_n, v_1\}$.



C_3 C_4 C_5 C_6

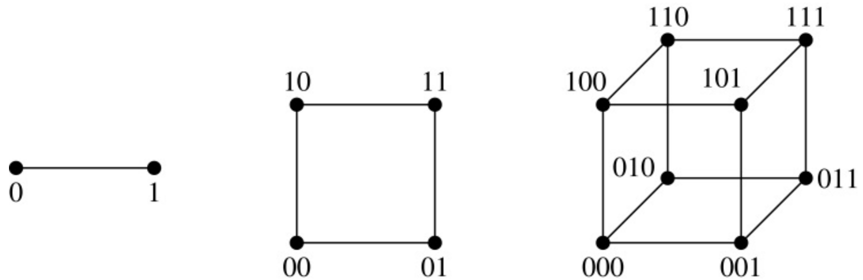
A *wheel* W_n is obtained by adding an additional vertex to a cycle C_n for $n \geq 3$ and connecting this new vertex to each of the n vertices in C_n by new edges.



W_3 W_4 W_5 W_6

Special Types of Simple Graphs: *n*-Cubes

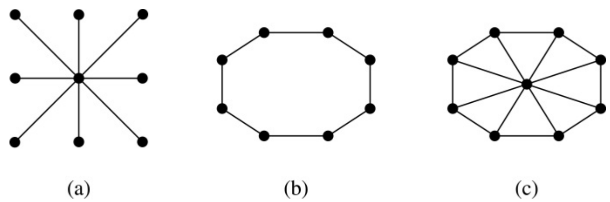
An *n-dimensional hypercube*, or *n-cube*, Q_n, is a graph with 2^n vertices representing all bit strings of length n, where there is an edge between two vertices that differ in exactly one bit position.



Q_1 Q_2 Q_3

Special Types of Graphs and Computer Network Architecture

Various special graphs play an important role in the design of computer networks.



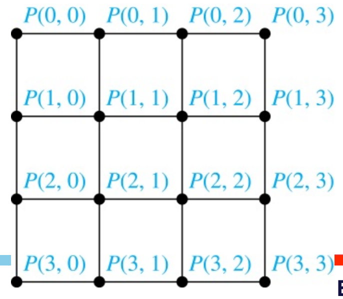
Some local area networks use a *star topology*, which is a complete bipartite graph $K_{1,n}$, as shown in (a). All devices are connected to a central control device.

Other local networks are based on a *ring topology*, where each device is connected to exactly two others using C_n, as illustrated in (b). Messages may be sent around the ring.

Others, as illustrated in (c), use a W_n – based topology, combining the features of a star topology and a ring topology.

Various special graphs also play a role in parallel processing where processors need to be interconnected as one processor may need the output generated by another.

- The *n-dimensional hypercube*, or *n-cube*, Q_n, is a common way to connect processors in parallel, e.g., Intel Hypercube.
- Another common method is the *mesh* network, illustrated here for 16 processors.

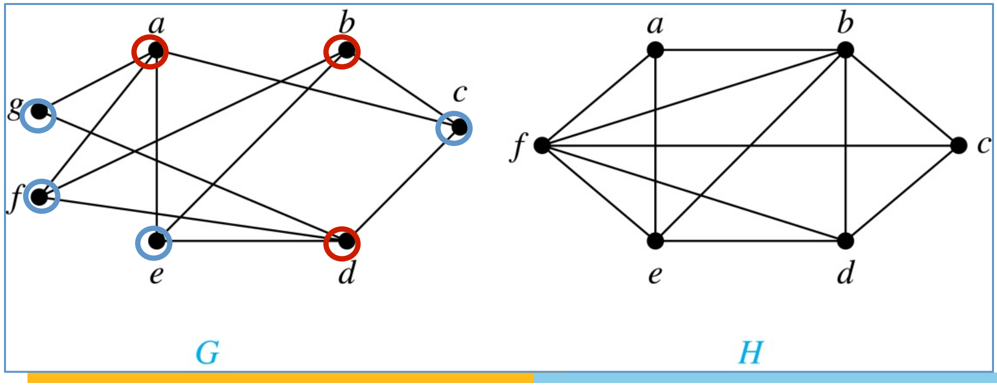


Bipartite Graphs

Definition: A simple graph G is bipartite if V can be partitioned into two disjoint subsets V_1 and V_2 such that every edge connects a vertex in V_1 and a vertex in V_2. In other words, there are no edges which connect two vertices in V_1 or in V_2.

It is not hard to show that an equivalent definition of a bipartite graph is a graph where it is possible to color the vertices red or blue so that no two adjacent vertices are the same color.

G is bipartite

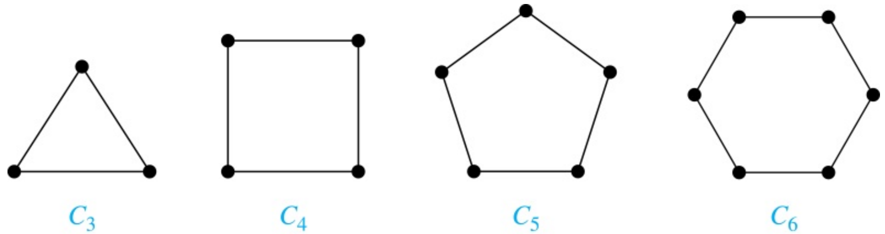


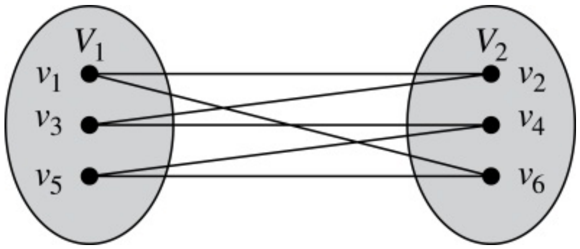
H is not bipartite since if we color *a* red, then the adjacent vertices *f* and *b* must both be blue.

Bipartite Graphs (*continued*)

Example: Show that C_6 is bipartite.

Solution: We can partition the vertex set into $V_1 = \{v_1, v_3, v_5\}$ and $V_2 = \{v_2, v_4, v_6\}$ so that every edge of C_6 connects a vertex in V_1 and V_2 .





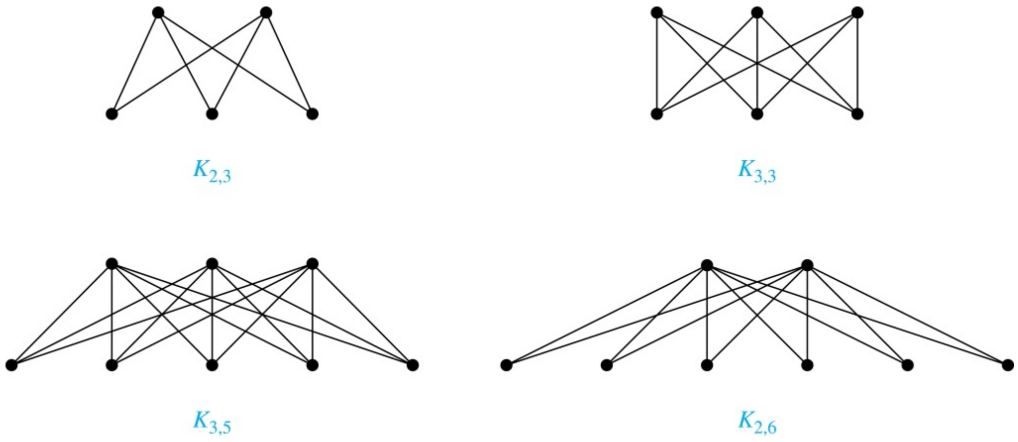
Example: Show that C_3 is not bipartite.

Solution: If we divide the vertex set of C_3 into two nonempty sets, one of the two must contain two vertices. But in C_3 every vertex is connected to every other vertex. Therefore, the two vertices in the same partition are connected. Hence, C_3 is not bipartite.

Complete Bipartite Graphs

Definition: A *complete bipartite graph* $K_{m,n}$ is a graph that has its vertex set partitioned into two subsets V_1 of size m and V_2 of size n such that there is an edge from every vertex in V_1 to every vertex in V_2.

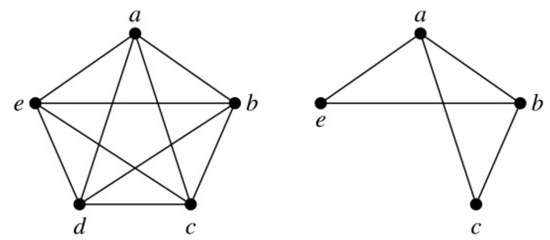
Example: We display four complete bipartite graphs here.



New Graphs from Old

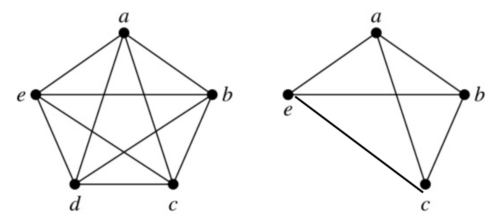
Definition: A *subgraph of a graph* $G = (V,E)$ is a graph (W,F), where $W \subset V$ and $F \subset E$. A subgraph H of G is a proper subgraph of G if $H \neq G$.

Example: Here we show K_5 and one of its subgraphs.



Definition: Let $G = (V, E)$ be a simple graph. The *subgraph induced* by a subset W of the vertex set V is the graph (W,F), where the edge set F contains an edge in E if and only if both endpoints are in W.

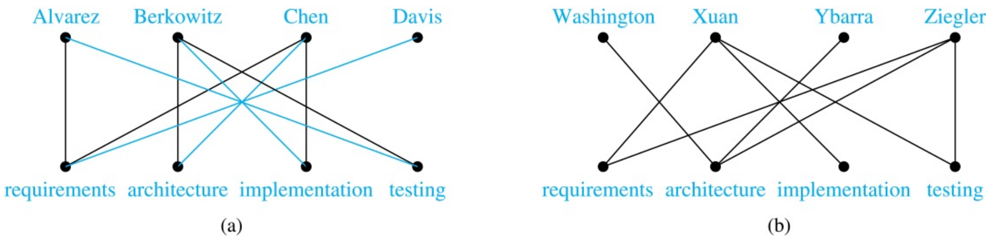
Example: Here we show K_5 and the subgraph induced by $W = \{a,b,c,e\}$.



Bipartite Graphs and Matchings

Bipartite graphs are used to model applications that involve matching the elements of one set to elements in another, for example:

Job assignments - vertices represent the jobs and the employees, edges link employees with those jobs they have been trained to do. A common goal is to match jobs to employees so that the most jobs are done.

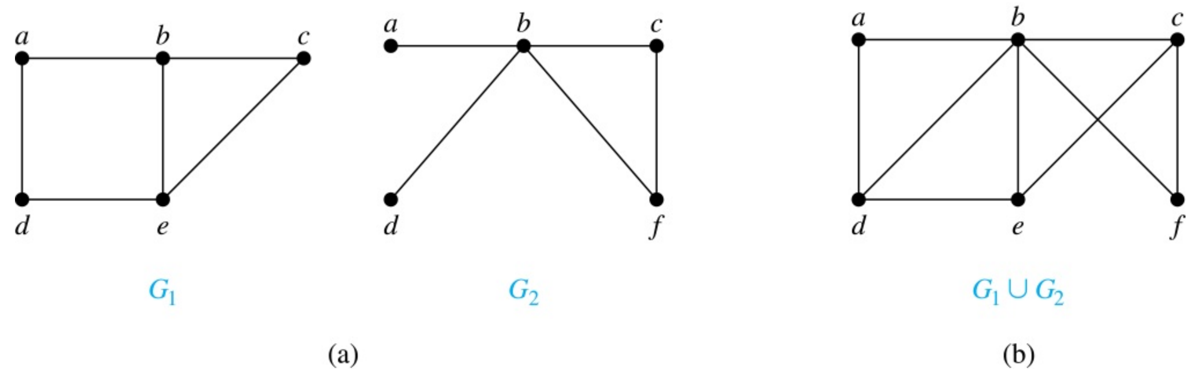


Marriage - vertices represent the men and the women and edges link a a man and a woman if they are an acceptable spouse. We may wish to find the largest number of possible marriages.

New Graphs from Old

Definition: The *union* of two simple graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is the simple graph with vertex set $V_1 \cup V_2$ and edge set $E_1 \cup E_2$. The union of G_1 and G_2 is denoted by $G_1 \cup G_2$.

Example:



Representing Graphs: Adjacency Lists

Definition: An *adjacency list* can be used to represent a graph with no multiple edges by specifying the vertices that are adjacent to each vertex of the graph.

Example:

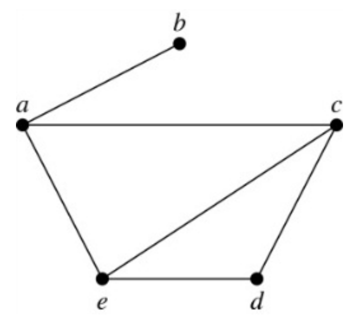


TABLE 1 An Adjacency List for a Simple Graph.

Vertex	*Adjacent Vertices*
a	b, c, e
b	a
c	a, d, e
d	c, e
e	a, c, d

Example:

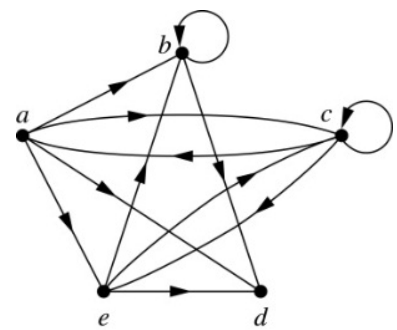


TABLE 2 An Adjacency List for a Directed Graph.

Initial Vertex	*Terminal Vertices*
a	b, c, d, e
b	b, d
c	a, c, e
d	
e	b, c, d

Adjacency Matrices

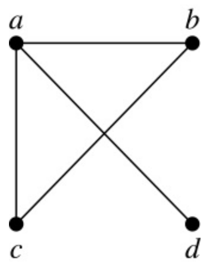
Definition: Suppose that $G = (V, E)$ is a simple graph where $|V| = n$. Arbitrarily list the vertices of G as $v_1, v_2, \ldots, v_n$. The *adjacency matrix* $\mathbf{A}_G$ of G, with respect to the listing of vertices, is the $n \times n$ zero-one matrix with 1 as its $(i, j)^{\text{th}}$ entry when v_i and v_j are adjacent, and 0 as its $(i, j)^{\text{th}}$ entry when they are not adjacent.

– In other words, if the graphs adjacency matrix is $\mathbf{A}_G = [a_{ij}]$, then

$$a_{ij} = \begin{cases} 1 & \text{if } \{v_i, v_j\} \text{ is an edge of } G, \\ 0 & \text{otherwise.} \end{cases}$$

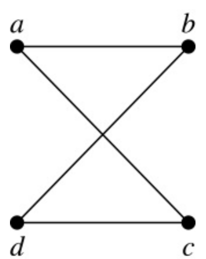
Adjacency Matrices (*continued*)

Example:



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

The ordering of vertices is a, b, c, d.



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

The ordering of vertices is a, b, c, d.

When a graph is sparse, that is, it has few edges relatively to the total number of possible edges, it is much more efficient to represent the graph using an adjacency list than an adjacency matrix. But for a dense graph, which includes a high percentage of possible edges, an adjacency matrix is preferable.

Note: The adjacency matrix of a simple graph is symmetric, i.e., $a_{ij} = a_{ji}$
Also, since there are no loops, each diagonal entry a_{ij} for $i = 1, 2, 3, \ldots, n$, is 0.

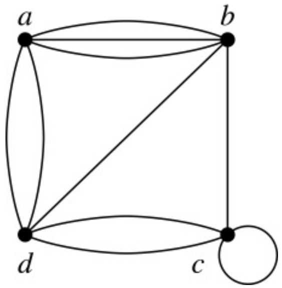
Adjacency Matrices (*continued*)

Adjacency matrices can also be used to represent graphs with loops and multiple edges.

A loop at the vertex v_i is represented by a 1 at the (i, j)th position of the matrix.

When multiple edges connect the same pair of vertices v_i and v_j, (or if multiple loops are present at the same vertex), the (i, j)th entry equals the number of edges connecting the pair of vertices.

Example: We give the adjacency matrix of the pseudograph shown here using the ordering of vertices a, b, c, d.



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

Adjacency Matrices (*continued*)

Adjacency matrices can also be used to represent directed graphs. The matrix for a directed graph $G = (V, E)$ has a 1 in its (i, j)th position if there is an edge from v_i to v_j, where $v_1, v_2, \ldots v_n$ is a list of the vertices.

- In other words, if the graphs adjacency matrix is $\mathbf{A}_G = [a_{ij}]$, then

$$a_{ij} = \begin{cases} 1 & \text{if } \{v_i, v_j\} \text{ is an edge of } G, \\ 0 & \text{otherwise.} \end{cases}$$

- The adjacency matrix for a directed graph does not have to be symmetric, because there may not be an edge from v_i to v_j, when there is an edge from v_j to v_i.

- To represent directed multigraphs, the value of a_{ij} is the number of edges connecting v_i to v_j.

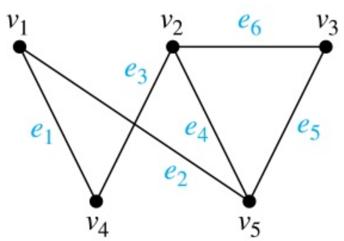
Representation of Graphs: Incidence Matrices

Definition: Let $G = (V, E)$ be an undirected graph with vertices where $v_1, v_2, \dots v_n$ and edges $e_1, e_2, \dots e_m$. The incidence matrix with respect to the ordering of V and E is the $n \times m$ matrix $\mathbf{M} = [m_{ij}]$, where

$$m_{ij} = \begin{cases} 1 & \text{when edge } e_j \text{ is incident with } v_i, \\ 0 & \text{otherwise.} \end{cases}$$

Incidence Matrices (*continued*)

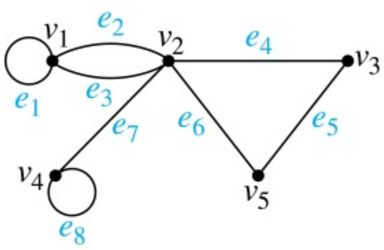
Example: Simple Graph and Incidence Matrix



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

The rows going from top to bottom represent v_1 through v_5 and the columns going from left to right represent e_1 through e_6.

Example: Pseudograph and Incidence Matrix



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

The rows going from top to bottom represent v_1 through v_5 and the columns going from left to right represent e_1 through e_8.