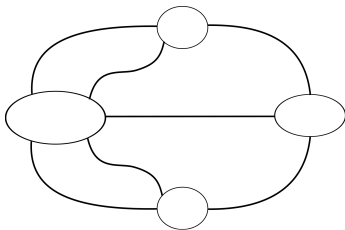


# Probabilistic Graphical Models: Principles and Applications

## Chapter 3: GRAPH THEORY

L. Enrique Sucar, INAOE



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# Graphs

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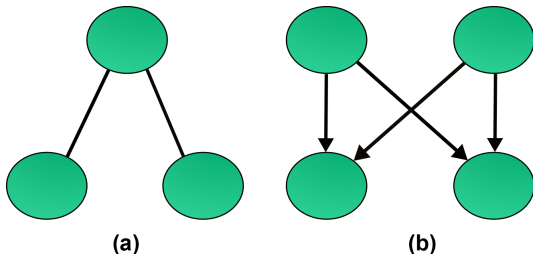
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- A *graph* provides a compact way to represent binary relations between a set of objects
- Objects are represented as circles or ovals, and relations as lines or arrows
- There are two basic types of graphs: *undirected graphs* and *directed graphs*



# Directed Graphs

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- A *directed graph* or *digraph* is an ordered pair,  $G = (V, E)$ , where  $V$  is a set of vertices or nodes and  $E$  is a set of arcs that represent a binary relation on  $V$
- Directed graphs represent anti-symmetric relations between objects, for instance the “parent” relation

# Undirected Graphs

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- An *undirected graph* is an ordered pair,  $G = (V, E)$ , where  $V$  is a set of vertices or nodes and  $E$  is a set of edges that represent symmetric binary relations:  
 $(V_j, V_k) \in E \rightarrow (V_k, V_j) \in E$
- Undirected graphs represent symmetric relations between objects, for example, the “brother” relation

# More Definitions

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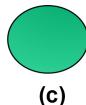
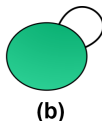
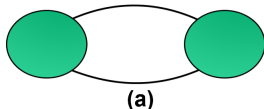
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- If there is an edge  $E_i(V_j, V_k)$  between nodes  $j$  and  $k$ , then  $V_j$  is adjacent to  $V_k$
- The *degree* of a node is the number of edges that are incident in that node
- Two edges associated to the same pair of vertices are said to be *parallel edges* (a)



# More Definitions

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- An edge that has its two endpoints in the same vertex is a *cycle* (b)
- A vertex that is not an endpoint to any edge is an *isolated vertex* –it has degree 0 (c)
- In a directed graph, the number of arcs pointing to a node is its *in degree*; and the number of edges pointing away from a node is its *out degree*

# Types of Graphs (I)

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**Chain graph:** a hybrid graph that has directed and undirected edges (a).

**Simple graph:** a graph that does not include cycles and parallel arcs (b).

**Multigraph:** a graph with several components (subgraphs), such that each component has no edges to the other components, i.e., they are disconnected (c).

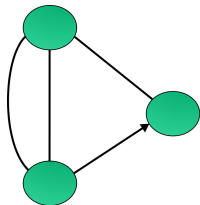
**Complete graph:** a graph that has an edge between each pair of vertices (d).

**Bipartite graph:** a graph in which the vertices are divided in two subsets,  $G_1$ ,  $G_2$ , such that all edges connect a vertex in  $G_1$  with a vertex in  $G_2$ ; that is, there are no edges between nodes in each subset (e).

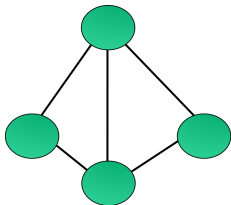
**Weighted graph:** a graph that has weights associated to its edges and/or vertices (f).



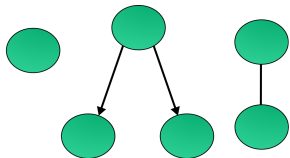
## Types of Graphs (II)



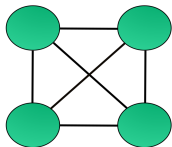
(a)



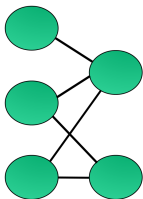
(b)



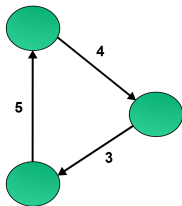
(c)



(d)



(e)



(f)

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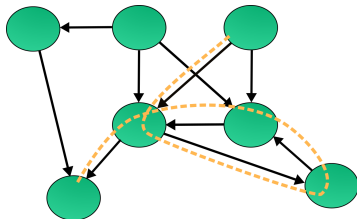
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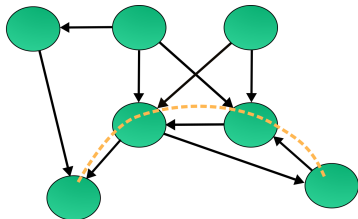
References

# Trajectories

- A *trajectory* is a sequence of edges,  $E_1, E_2, \dots, E_n$  such that the final vertex of each edge coincides with the initial vertex of the next edge in the sequence
- A *simple* trajectory (a) does not include the same edge two or more times; an *elemental* trajectory (b) is not incident on the same vertex more than once



(a)



(b)

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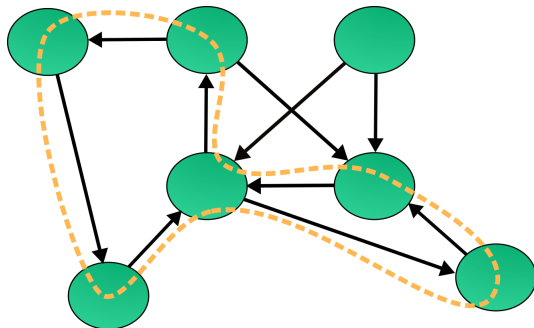
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# Circuits

- A *circuit* is a trajectory such that the final vertex coincides with the initial one
- A *simple* circuit does not include the same edge two or more times; an *elemental* circuit is not incident on the same vertex more than once (except the initial/final vertex)



# Directed Acyclic Graphs

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- A Directed Acyclic Graph (DAG) is a directed graph that has no directed circuits (a directed circuit is a circuit in which all edges in the sequence follow the directions of the arrows)

# Some Problems on Graphs

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- Finding a trajectory that includes all edges in a graph only once (Euler trajectory).
- Finding a circuit that includes all edges in a graph only once (Euler circuit).
- Finding a trajectory that includes all vertices in a graph only once (Hamiltonian trajectory).
- Finding a circuit that includes all vertices in a graph only once (Hamiltonian circuit).
- Finding a Hamiltonian circuit in a weighted graph with minimum cost (Traveling salesman problem)<sup>1</sup>.

---

<sup>1</sup>In this case the nodes represent cities and the edges roads with an associated distance or time, so the solution will provide a traveling salesman with the “best” (minimum distance or time) route to cover all the cities.

# Isomorphism (I)

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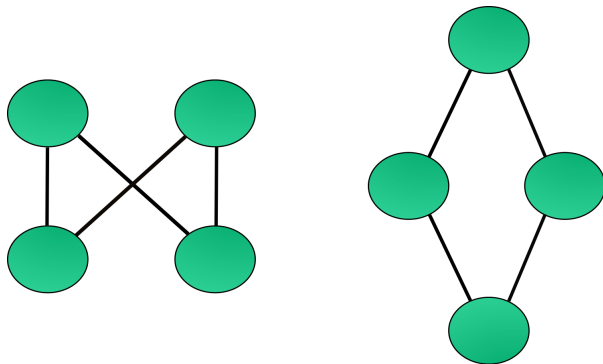
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- Two graphs are isomorphic if there is a one to one correspondence between their vertices and edges, so that the incidences are maintained
- Types:
  - ① *Graph isomorphism.* Graphs  $G_1$  and  $G_2$  are isomorphic.
  - ② *Subgraph isomorphism.* Graph  $G_1$  is isomorphic to a subgraph of  $G_2$  (or vice versa).
  - ③ *Double subgraph isomorphism.* A subgraph of  $G_1$  is isomorphic to a subgraph of  $G_2$ .

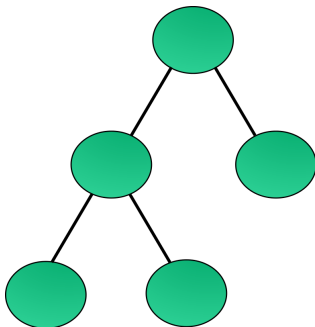
## Isomorphism (II)



- Determining if two graphs are isomorphic (type 1) is an NP problem; while the subgraph and double subgraph isomorphism problems (type 2 and 3) are NP-complete

# Undirected trees

- An undirected tree is a connected graph that does not have simple circuits
- There are two classes of vertices or nodes in an undirected tree: (i) leaf or terminal nodes, with degree one; (ii) internal nodes, with degree greater than one



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# Properties

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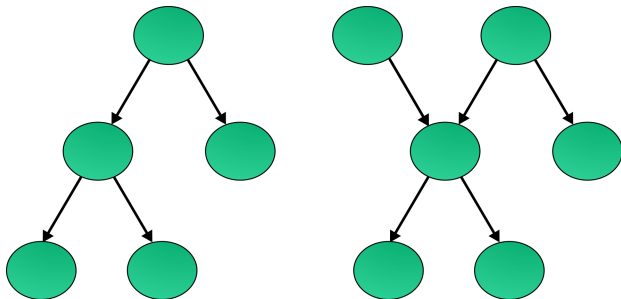
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- There is a simple trajectory between each pair of vertices.
- The number of vertices,  $|V|$ , is equal to the number of edges,  $|E|$  plus one:  $|V| = |E| + 1$ .
- A tree with two or more vertices has at least two leaf nodes.

## Directed trees

- A directed tree is a connected directed graph such that there is only a single directed trajectory between each pair of nodes
- A rooted tree has a single node with an in degree of zero (the root node) and the rest have in degree of one
- A polytree might have more than one node with in degree zero (roots), and certain nodes (zero or more) with in degree greater than one



# Terminology (I)

**Root:** a node with in degree equal to zero.

**Leaf:** a node with out degree equal to zero.

**Internal node:** a node with out degree greater than zero.

**Parent / Child:** if there is a directed arc from  $A$  to  $B$ ,  $A$  is parent of  $B$  and  $B$  is a child of  $A$ .

**Brothers:** two or more nodes that have the same parent.

**Ascendants / Descendants:** if there is a directed trajectory from  $A$  to  $B$ ,  $A$  is an ascendant of  $B$  and  $B$  is a descendant of  $A$ .

**Subtree with root  $A$ :** a subtree with  $A$  as its root.

**Subtree of  $A$ :** a subtree with a child of  $A$  as its root.

**K-ary Tree:** a tree in which each internal node has at most  $K$  children. It is a regular tree if each internal node has  $K$  children.

**Binary Tree:** a tree in which each internal node has at most two children.

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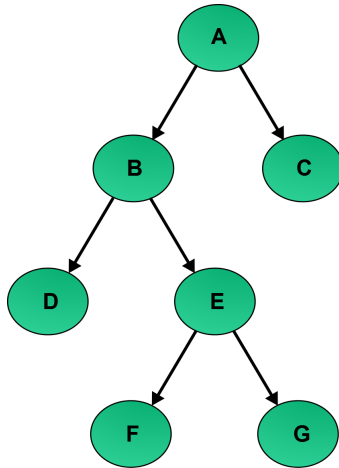
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# Terminology (II)



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# Complete set and subsets

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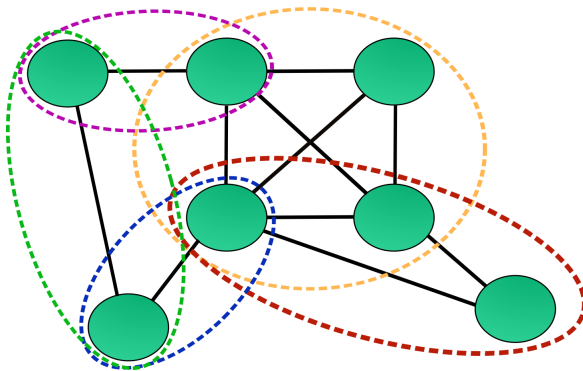
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- A *complete graph* is a graph,  $G_C$ , in which each pair of nodes is adjacent; that is, there is an edge between each pair of nodes
- A *complete set*,  $W_C$  is a subset of  $G$  that induces a complete subgraph of  $G$ . It is a subset of vertices of  $G$  so that each pair of nodes in this subgraph is adjacent

# Cliques

- A *clique*,  $C$ , is a subset of graph  $G$  such that it is a complete set that is maximal; that is, there is no other complete set in  $G$  that contains  $C$



# Ordering

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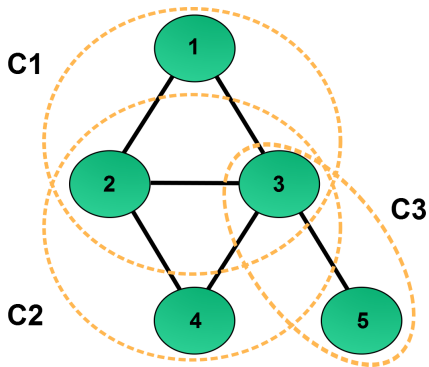
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- An ordering of the nodes in a graph consists in assigning an integer to each vertex
- Given a graph  $G = (V, E)$ , with  $n$  vertices, then  $\alpha = [V_1, V_2, \dots, V_n]$  is an ordering of the graph;  $V_i$  is *before*  $V_j$  according to this ordering, if  $i < j$
- An ordering  $\alpha$  of a graph  $G = (V, E)$  is a *perfect ordering* if all the adjacent vertices of each vertex  $V_i$  that are before  $V_i$ , according to this ordering, are completely connected

# Perfect Ordering



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# Clique Ordering

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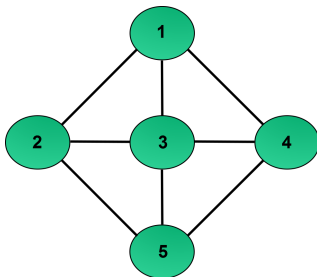
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- In an analogous way as an ordering of the nodes, we can define an ordering of the cliques,  
$$\beta = [C_1, C_2, \dots, C_p]$$
- An ordering  $\beta$  of the cliques has the *running intersection property*, if all the common nodes of each clique  $C_i$  with previous cliques according to this order are contained in a clique  $C_j$ ;  $C_j$  is the *parent* of  $C_i$
- It is possible that a clique has more than one parent

## Triangulated graphs

- A graph  $G$  is *triangulated* if every simple circuit of length greater than three in  $G$  has a chord
- A chord is an edge that connects two of the vertices in the circuit and that is not part of that circuit
- A condition for achieving a perfect ordering of the vertices, and having an ordering of the cliques that satisfies the running intersection property, is that the graph is triangulated



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# Maximum Cardinality Search

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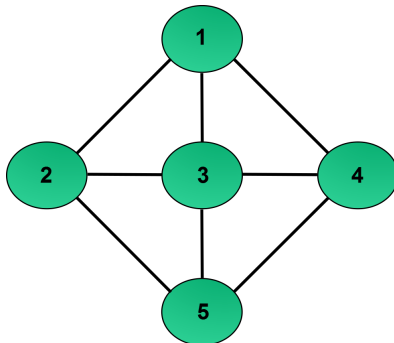
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- Given that a graph is triangulated, the following algorithm guarantees a perfect ordering:
  - 1 Select any vertex from  $V$  and assign it number 1.
  - 2 WHILE Not all vertices in  $G$  have been numbered:
    - 1 From all the non-labeled vertices, select the one with higher number of adjacent labeled vertices and assign it the next number.
    - 2 Break ties arbitrarily.

# Example - Maximum Cardinality Search



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# Graph filling

- The filling of a graph consists of adding arcs to an original graph  $G$  to make it triangulated
- The following algorithm makes the graph triangulated:
  - ① Order the vertices  $V$  with maximum cardinality search:  $V_1, V_2, \dots, V_n$ .
  - ② FOR  $i = n$  TO  $i = 1$ 
    - ① For node  $V_i$ , select all its adjacent nodes  $V_j$  such that  $j > i$ . Call this set of nodes  $A_i$ .
    - ② Let  $V_m$  be the node with largest number in  $A_i$
    - ③ Add an arc from  $V_i$  to  $V_k$  if  $k > i$ ,  $k < m$  and  $V_k \notin A_i$ .

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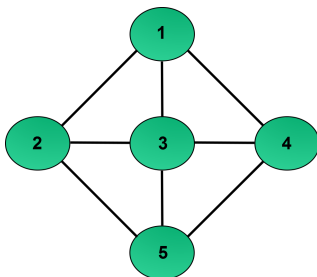
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## Example - Graph Filling



$A_5: \emptyset$

$A_4: 5$

$A_3: 4, 5$

$A_2: 3, 5$ . An arc is added from 2 to 4.

$A_1: 2, 3, 4$ .

The resulting graph has one additional arc: 2 – 4

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# Additional Reading

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