AMRITA VISHWA VIDYAPEETHAM
DEEMED TO BE UNIVERSITY

22BIO211: Intelligence of Biological Systems - 2

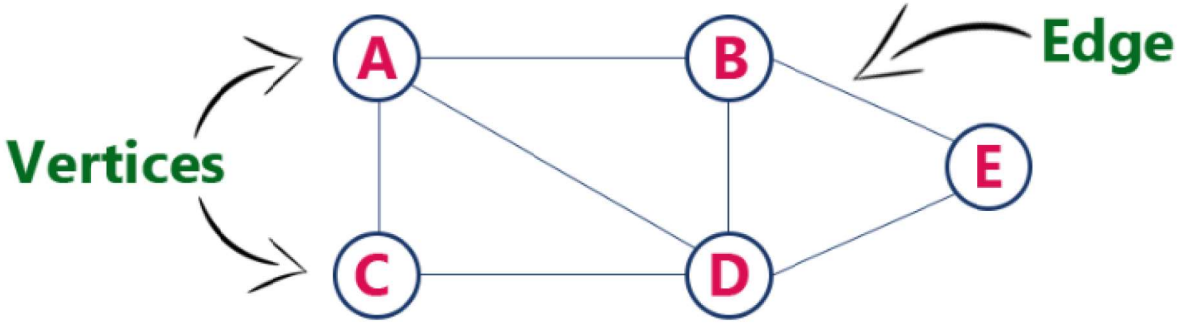
INTRODUCTION TO GRAPHS

Dr. Manjusha Nair M
Amrita School of Computing, Amrita Vishwa Vidyapeetham
Email : manjushanair@am.amrita.edu
Contact No: 9447745519

Graphs

- Graph is a non-linear data structure consisting of a collection of vertices (nodes) and arcs(edges) in which vertices (nodes) are connected with arcs(edges)

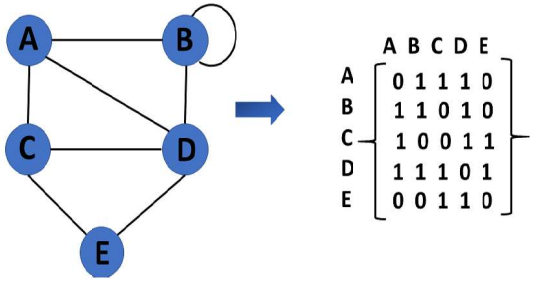
Generally, a graph **G** is represented as **G = (V , E)**, where **V is set of vertices** and **E is set of edges**.



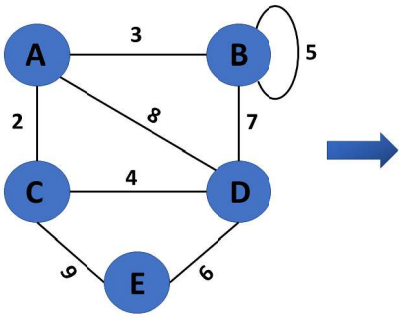
The given graph has 5 vertices and 7 edges.
V = {A,B,C,D,E}
E = {(A,B),(A,C)(A,D),(B,D),(C,D),(B,E),(E,D)}.

Graphs

- If we represent a list of cities using a graph
  - the vertices would represent the cities.
  - the edges would represent the path between the cities.
- Edges can represent the relationship between vertices
  - in the form of simply [1, 0] whether there is a connection or not
  - or a given weight that may represent values such as distance, the strength of the relationship or the number of times they interact.



	A	B	C	D	E
A	0	1	1	1	0
B	1	1	0	1	0
C	1	0	0	1	1
D	1	1	1	0	1
E	0	0	1	1	0



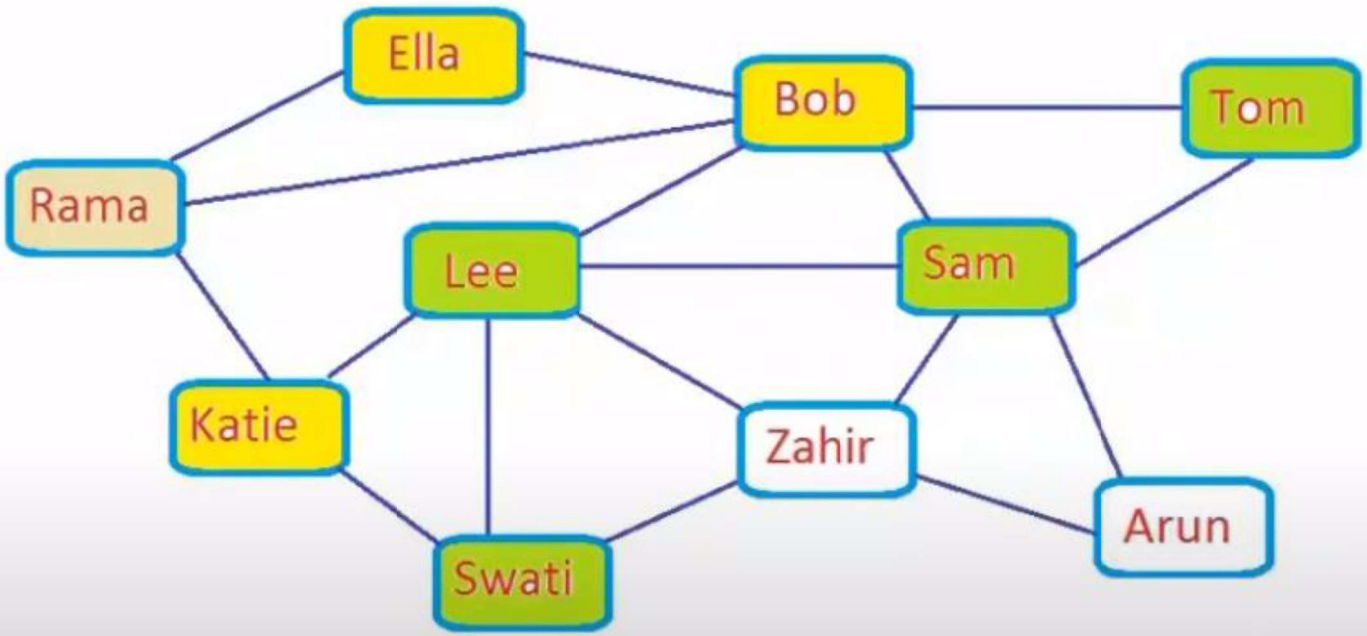
	A	B	C	D	E
A	0	3	2	8	0
B	3	5	0	7	0
C	2	0	0	4	9
D	8	7	4	0	6
E	0	0	9	6	0

Applications of Graphs

- Graphs are used everywhere
  - To visualize organized data.
  - Directed Graphs are used in Google's Page Ranking Algorithm.
  - Social Networks use graphs to represent different users as vertices and edges to represent the connections between them.
  - In a mapping application, graphs are used to represent places and the path (distance) between them.
  - modelling Computer Networks.

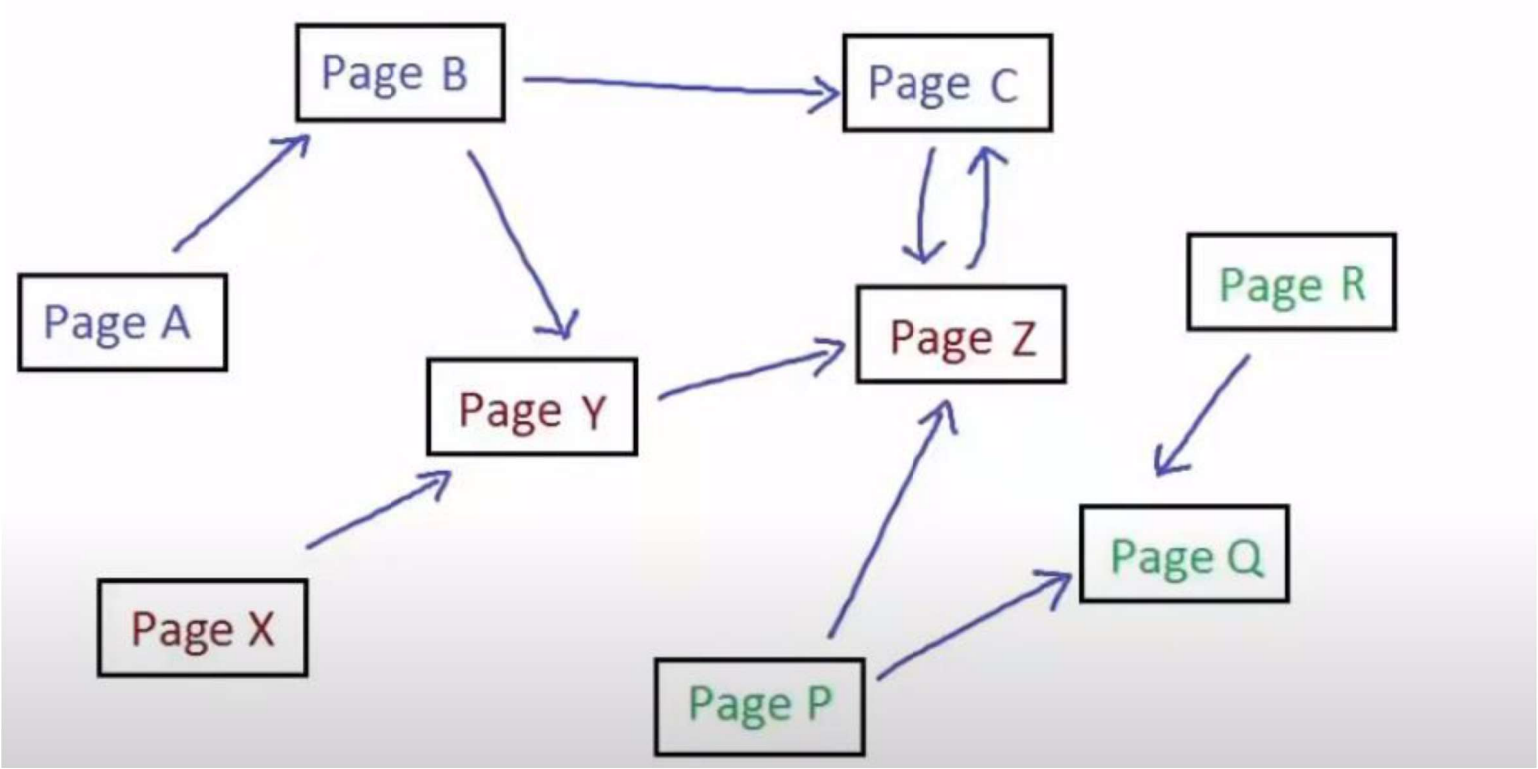
Some Applications of Graphs

Social Network: Undirected Graph



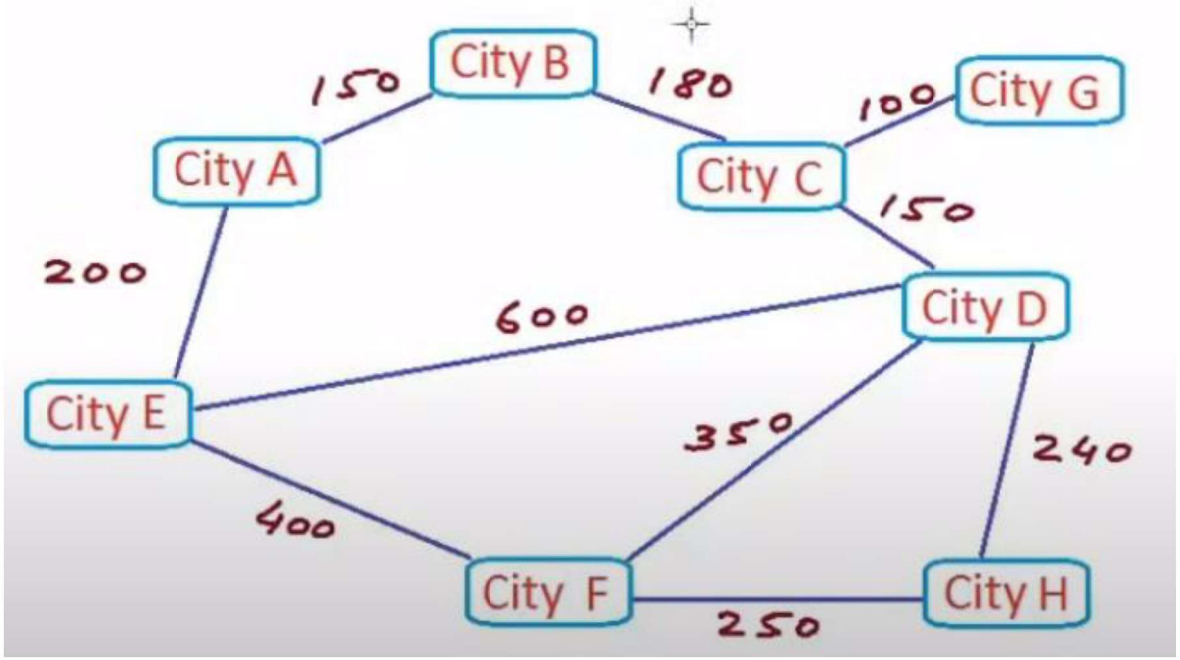
Some Applications of Graphs

World Wide Web: Directed Graph

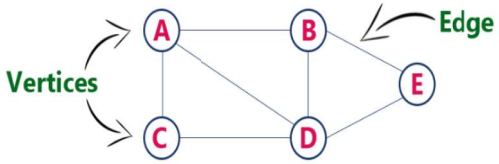


Some Applications of Graphs

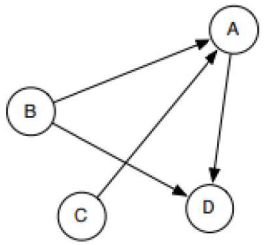
Intercity Road Network: Weighted Graph



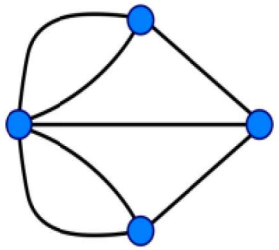
Important Terminologies

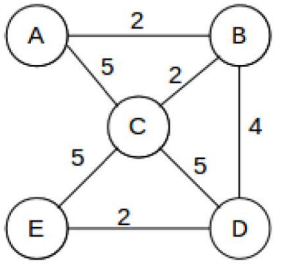


- Vertex/node – data element
- Edge/arc – connecting link
  - Undirected
  - Directed
  - Weighted
- Undirected Graph
- Directed Graph
- Mixed Graph
- Degree: number of edges connected to a vertex
  - Indegree : incoming edges
  - Outdegree: outgoing edges



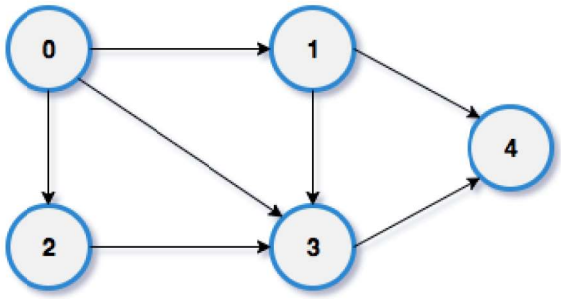
directed graph

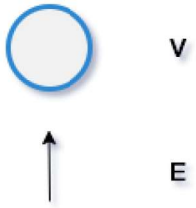

undirected graph



weighted graph

Important Terminologies





In-degree

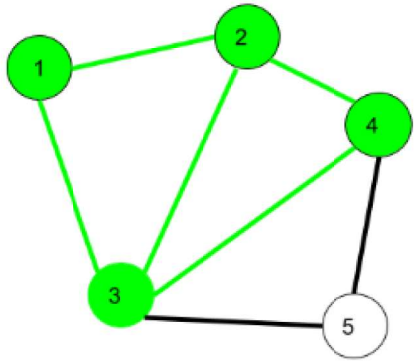
In-degree of vertex 0 = 0
In-degree of vertex 1 = 1
In-degree of vertex 2 = 1
In-degree of vertex 3 = 3
In-degree of vertex 4 = 2

out-degree

Out-degree of vertex 0 = 3
Out-degree of vertex 1 = 2
Out-degree of vertex 2 = 1
Out-degree of vertex 3 = 1
Out-degree of vertex 4 = 0

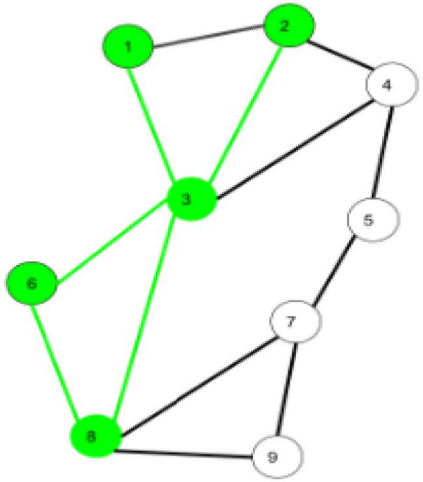
Important Terminologies

- Walk : A sequence of edges which joins a sequence of vertices.
  - Vertices and edges can be repeated
- Trail : A walk in which all edges are distinct (vertex can be repeated)
- Circuit : Closed Trail.



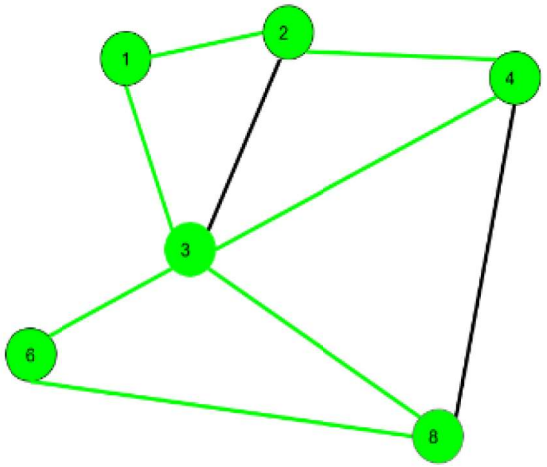
Walk

1->2->3->4->2->1->3



Trail

1->3->8->6->3->2

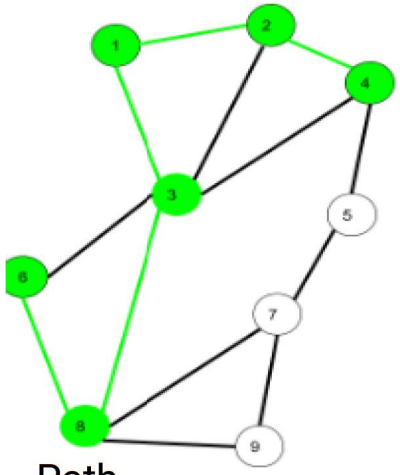


Circuit

1->2->4->3->6->8->3->1

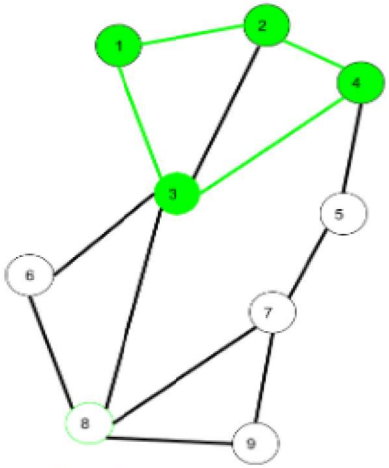
Important Terminologies

- Path: A trail in which all vertices are distinct (Both vertices and edges are not repeated)
- Cycle : A trail in which only repeated vertices are the first and last vertices.



Path

6->8->3->1->2->4



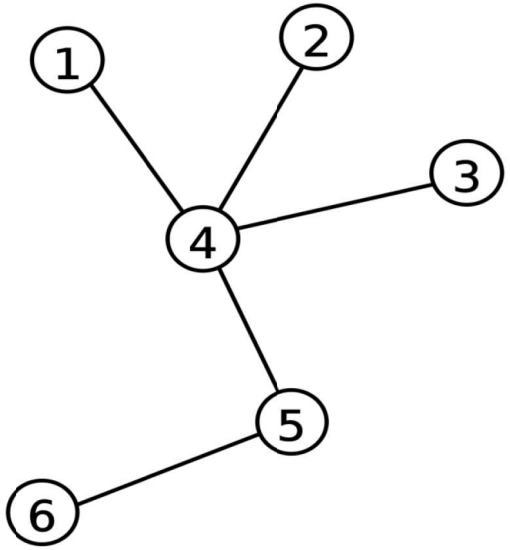
Cycle

1->2->4->3->1

1.Walk : Vertices may repeat. Edges may repeat (Closed or Open)
2.Trail : Vertices may repeat. Edges cannot repeat (Open)
3.Circuit : Vertices may repeat. Edges cannot repeat (Closed)
4.Path : Vertices cannot repeat. Edges cannot repeat (Open)
5.Cycle : Vertices cannot repeat. Edges cannot repeat (Closed)

Special Graphs

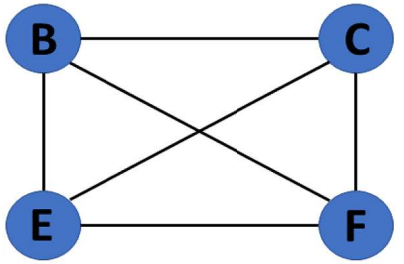
- **Tree**
  - An undirected graph with zero cycles is called a tree.
    - A cycle in a graph is a sequence with the first and last vertices in the repeating sequence.



Special Graphs

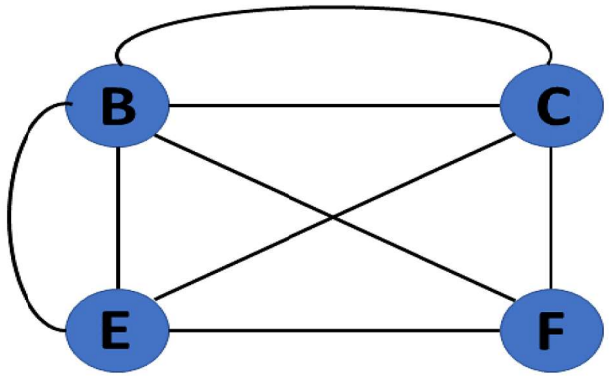
- **Trivial Graph**
  - A graph G= (V, E) is trivial if it contains only a single vertex and no edges.

- **Simple Graph**
  - If each pair of nodes or vertices in a graph G=(V, E) has only one edge, it is a simple graph.
  - As a result, there is just one edge linking two vertices, depicting one-to-one interactions between two elements.



Special Graphs

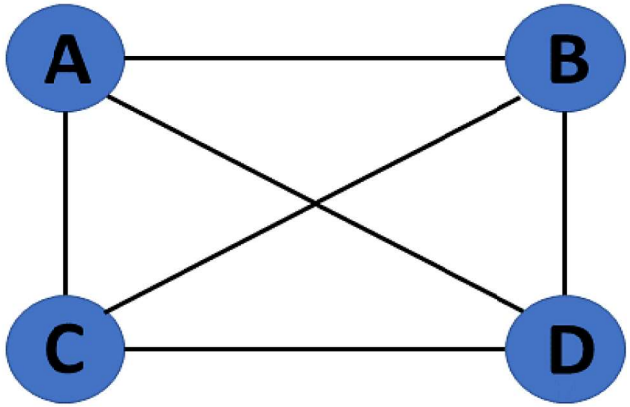
- **Multi Graph**
  - If there are numerous edges between a pair of vertices in a graph G= (V, E), the graph is referred to as a multigraph. There are no self-loops in a Multigraph.

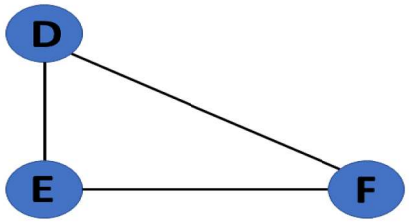


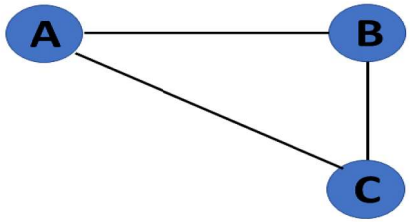
Special Graphs

- **Connected Graph**
  - If there is a path between one vertex of a graph data structure and any other vertex, the graph is connected.

- **Disconnected Graph**
  - When there is no edge linking some of the vertices, the graph is disconnected



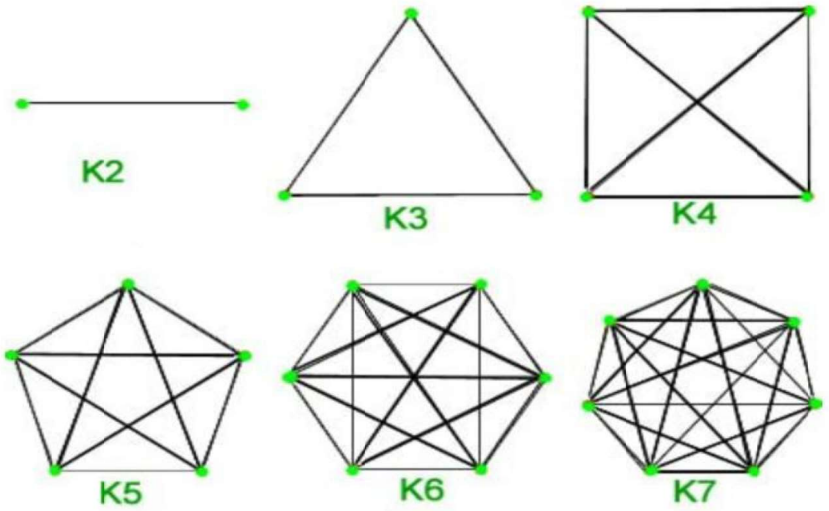




Special Graphs

- **Complete Graphs**

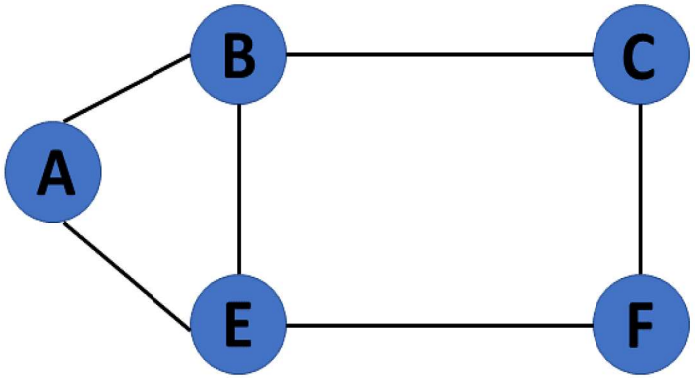
- Complete graphs have a unique edge between every pair of vertices.
- A complete graph n vertices have (n*(n-1)) / 2 edges



Special Graphs

- **Cyclic Graphs**

- If a graph contains at least one graph cycle, it is considered to be cyclic.

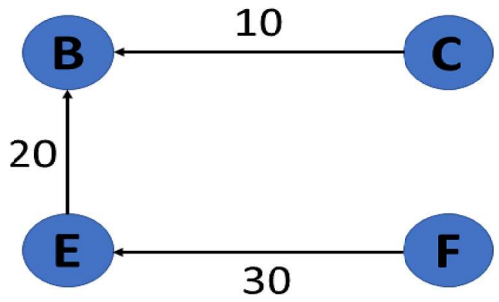


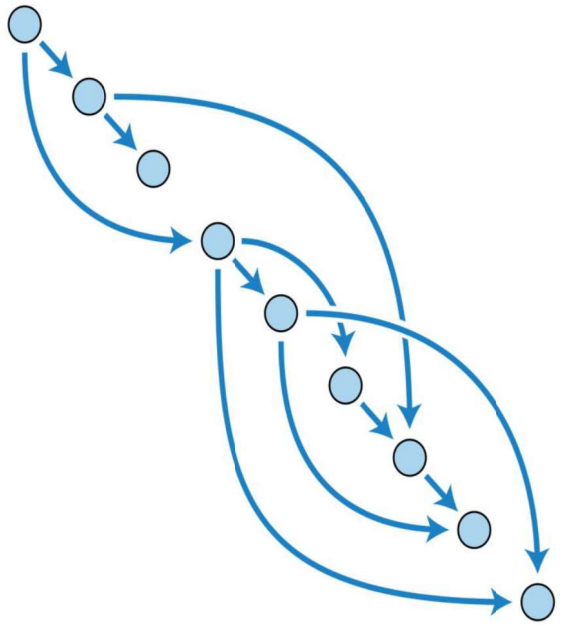
- **Acyclic Graphs**

- When there are no cycles in a graph, it is called an acyclic graph.

Special Graphs

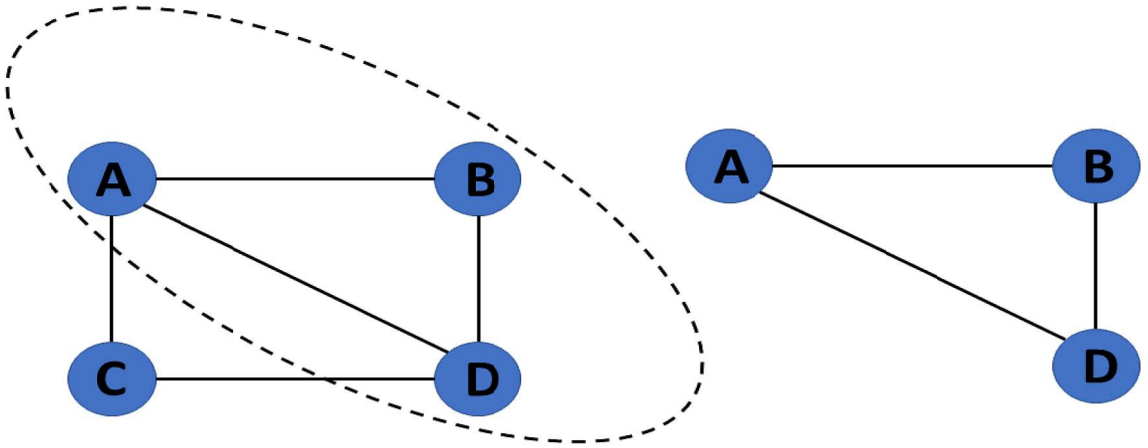
- **Directed Acyclic Graphs (DAG)**
- A graph with directed edges but no cycle.
- That is, it consists of vertices and edges with each edge directed from one vertex to another, such that following those directions will never form a closed loop.
- They represent structures with dependencies
- DAGs are used by compilers to represent expressions and relationships in a program.





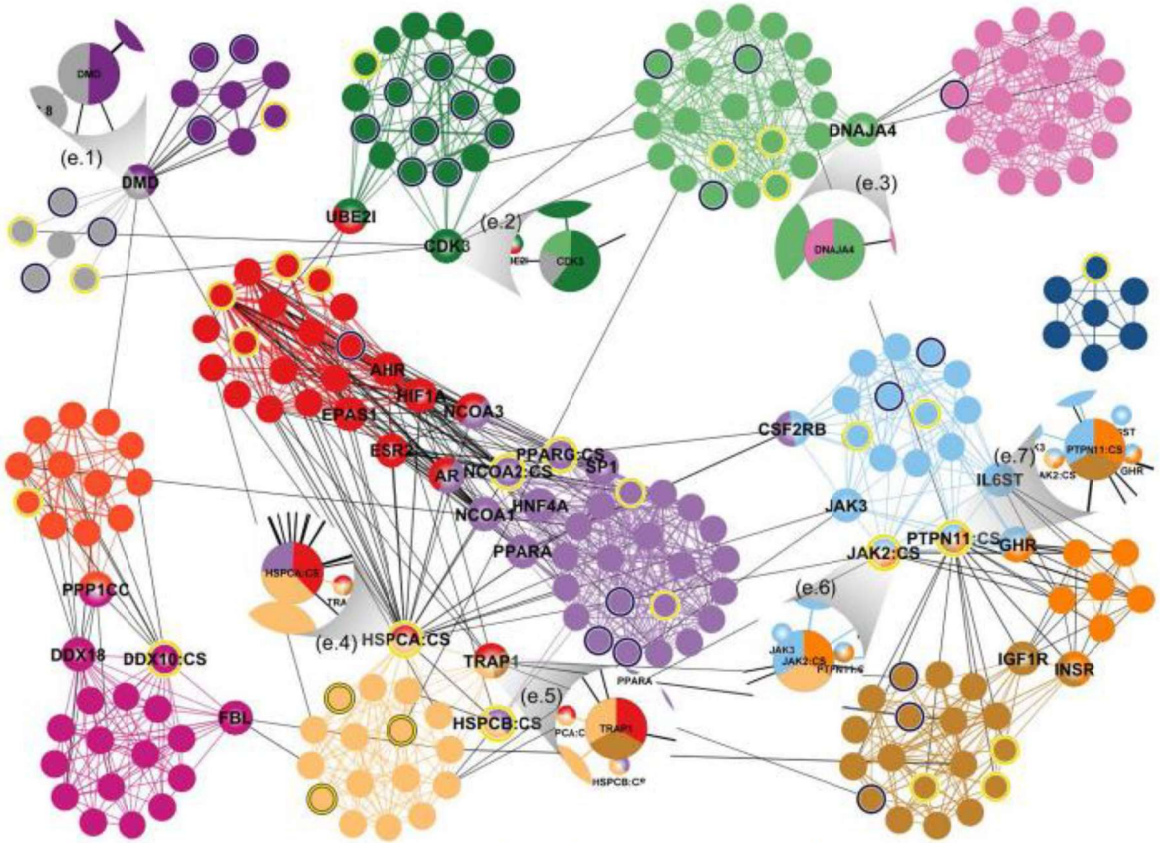
Special Graphs

- **Sub Graphs**
  - The vertices and edges of a graph that are subsets of another graph are known as a subgraph.



Applications of Graphs : Biological and Biomedical Networks

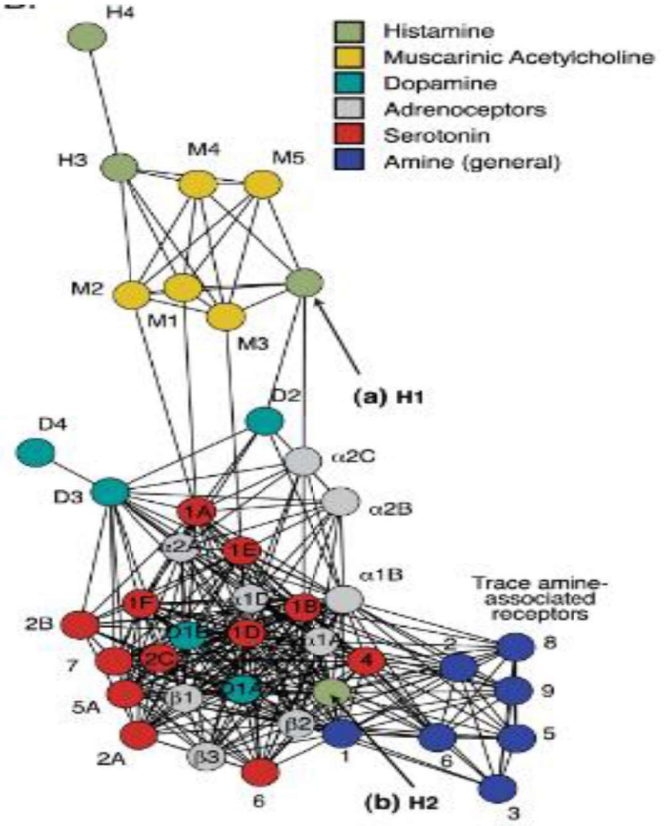
- Protein-Protein Interaction Networks (PPIs)
  - *information about how different proteins operate with each other to enable a biological process within a cell.*



Protein-protein-interaction network comprising 1,253 weighted interactions between 232 proteins.

Applications of Graphs : Biological and Biomedical Networks

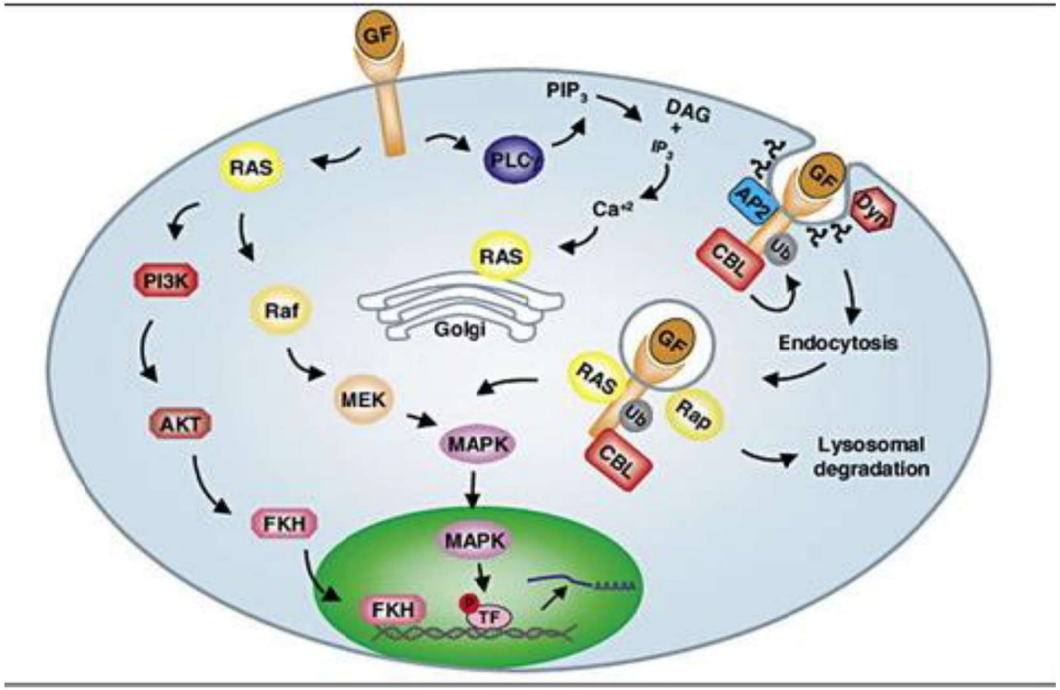
- Sequence Similarity Networks (SSNs)
  - *Nodes representing proteins or genes and edges capturing the sequence similarity between amino acid or nucleotide sequences.*



Sequence Similarity network describing the interrelationships of 42 amine-binding human GPCR domain

Applications of Graphs : Biological and Biomedical Networks

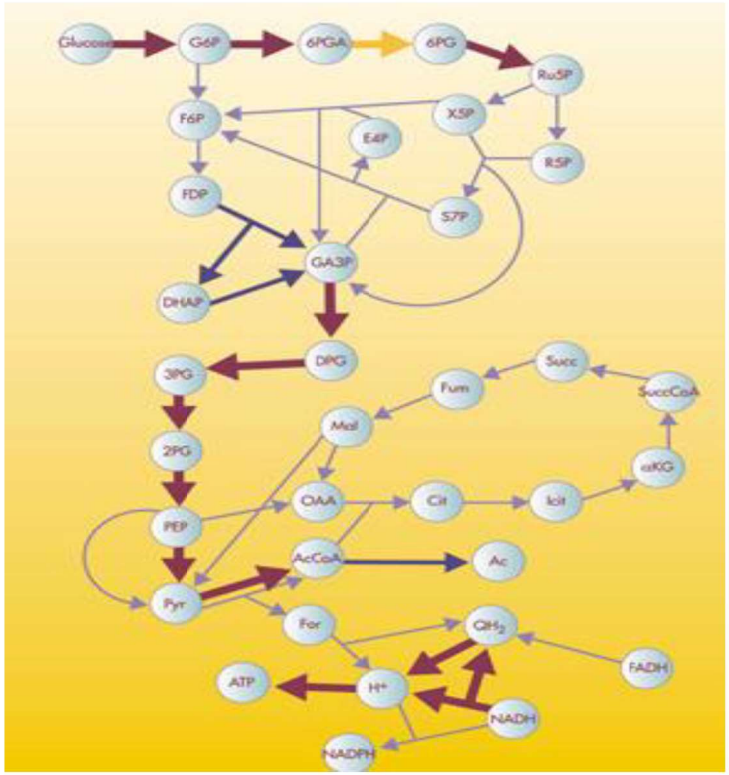
- Signal Transduction Networks(STNs)
  - *The transmission of molecular signals and a series of molecular events within a cell or from the exterior to its interior*



Signal Transduction of Intracellular Biochemical Pathways in response to extracellular cues

Applications of Graphs : Biological and Biomedical Networks

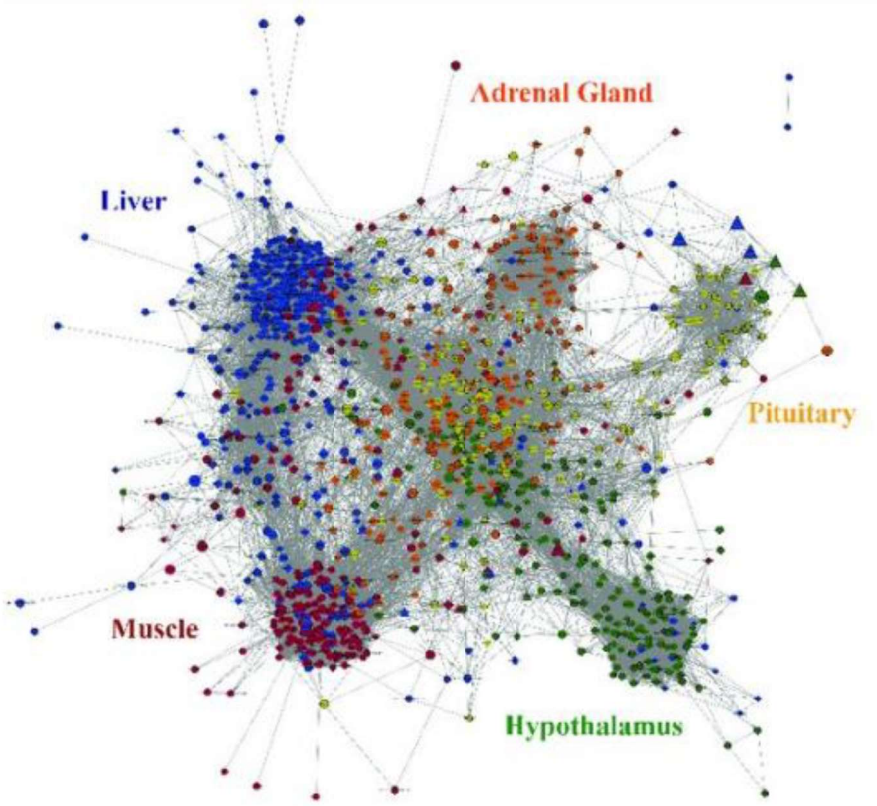
- Metabolic Networks (MNs)
  - *showing interactions between enzymes and metabolites (aminoacids/poly saccharides)*



Metabolic network model for Escherichia coli.

Applications of Graphs : Biological and Biomedical Networks

- Gene Co-expression Networks
  - *two nodes (genes) are connected if there is a significant co-expression between them.*



Gene co- expression network constructed on 1,335 selected genes

Summary

- Graphs
- Applications of Graphs
- Important terminologies
- Special Graphs