BACKGROUND: A BRIEF INTRODUCTION TO GRAPH THEORY

- **General definitions; Representations;**
- **Graph Traversals;**
- **Topological sort;**

Graphs – definitions & representations

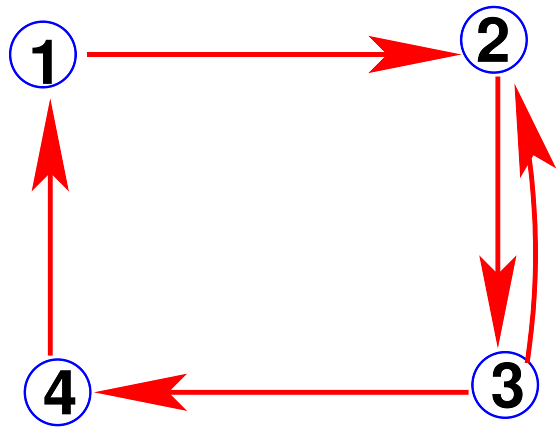
➤ Graph theory is a fundamental tool in sparse matrix techniques.

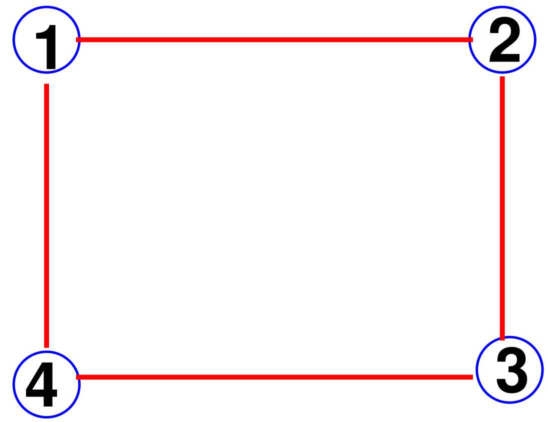
DEFINITION. A graph G is defined as a pair of sets $G = (V, E)$ with $E \subset V \times V$. So G represents a binary relation. The graph is undirected if the binary relation is symmetric. It is directed otherwise. V is the vertex set and E is the edge set.

If R is a binary relation between elements in V then, we can represent it by a graph $G = (V, E)$ as follows:

$$(u, v) \in E \leftrightarrow u\ R\ v$$

Undirected graph $\leftrightarrow$ symmetric relation





(1 R 2); (4 R 1); (2 R 3); (3 R 2); (3 R 4)

(1 R 2); (2 R 3); (3 R 4); (4 R 1)

Given the numbers 5, 3, 9, 15, 16, show the two graphs representing the relations

R1: Either $x < y$ or y divides x.

R2: x and y are congruent modulo 3. [mod(x,3) $=$ mod(y,3)]

- $|E| \le |V|^2$. For undirected graphs: $|E| \le |V|(|V|+1)/2$.
- A sparse graph is one for which $|E| \ll |V|^2$.

Graphs – Examples and applications

➤ Applications of graphs are numerous.

1. Airport connection system: (a) R (b) if there is a non-stop flight from (a) to (b).

2. Highway system;

3. Computer Networks;

4. Electrical circuits;

5. Traffic Flow;

6. Sparse matrix computations;

...

Basic Terminology & notation:

- If $(u, v) \in E$, then v is adjacent to u. The edge (u, v) is incident to u and v.
- If the graph is directed, then (u, v) is an outgoing edge from u and incoming edge to v
- $Adj(i) = \{j | j \text{ adjacent to } i\}$
- The degree of a vertex v is the number of edges incident to v. Can also define the indegree and outdegree. (Sometimes self-edge $i \rightarrow i$ omitted)
- $|S|$ is the cardinality of set S [so $|Adj(i)| ==$ deg(i)]
- A subgraph $G' = (V', E')$ of G is a graph with $V' \subset V$ and $E' \subset E$.

Representations of Graphs

➤ A graph is nothing but a collection of vertices (indices from 1 to n), each with a set of its adjacent vertices [in effect a 'sparse matrix without values']

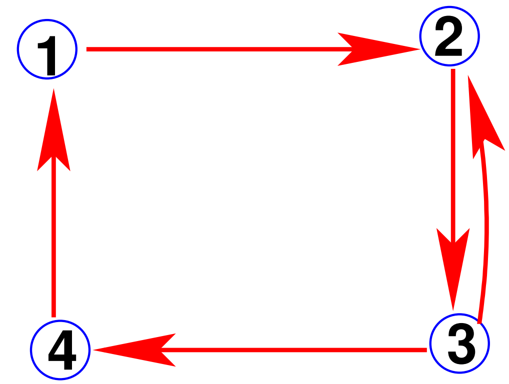
➤ Therefore, can use any of the sparse matrix storage formats - omit the real values arrays.

Adjacency matrix Assume $V = \{1, 2, \cdots, n\}$. Then the adjacency matrix of $G = (V, E)$ is the $n \times n$ matrix, with entries:

$$a_{i,j} = \begin{cases} 1 \text{ if } (i,j) \in E \\ 0 \text{ Otherwise} \end{cases}$$

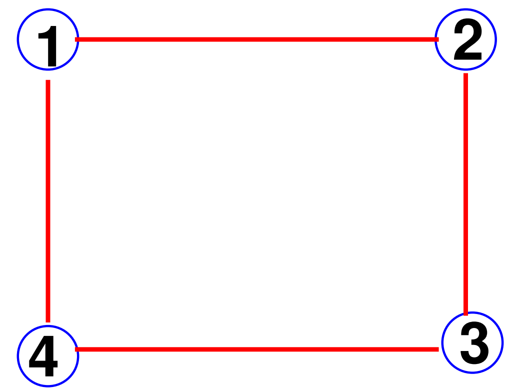
Representations of Graphs (cont.)

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

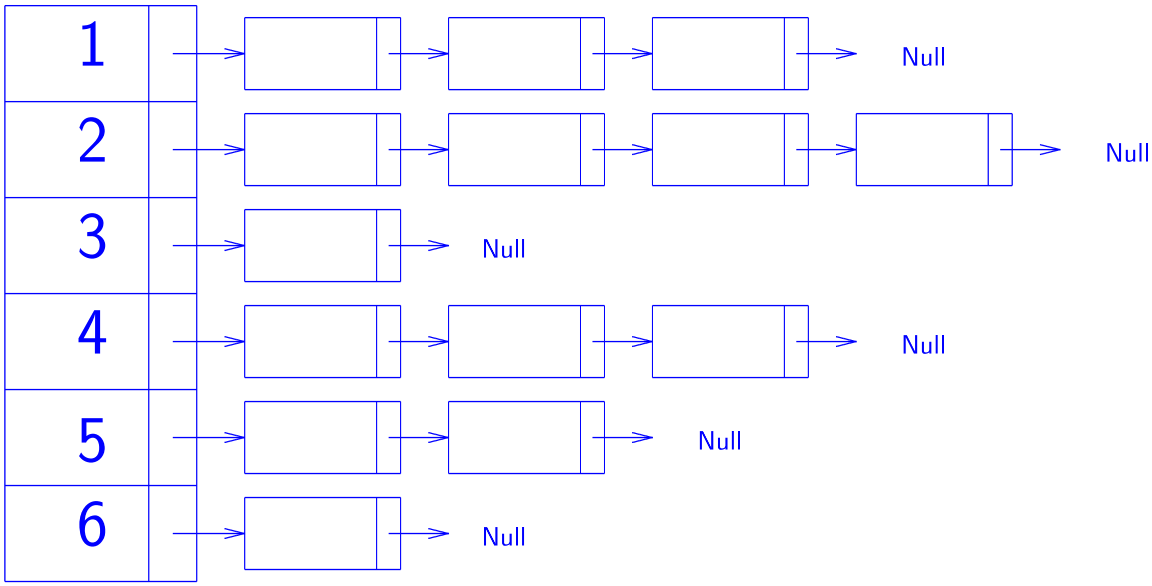


Example:

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



Dynamic representation: Linked lists



- An array of linked lists. A linked list associated with vertex i, contains all the vertices adjacent to vertex i.
- General and concise for 'sparse graphs' (the most practical situations).
- Not too economical for use in sparse matrix methods

More terminology & notation

- For a given $Y \subset X$, the section graph of Y is the subgraph $G_Y = (Y, E(Y))$ where

$$E(Y) = \{(x, y) \ \in \ E | x \ \in \ Y, \quad y \ \ in \, Y\}$$

- A section graph is a clique if all the nodes in the subgraph are pairwise adjacent ($\longrightarrow$ dense block in matrix)

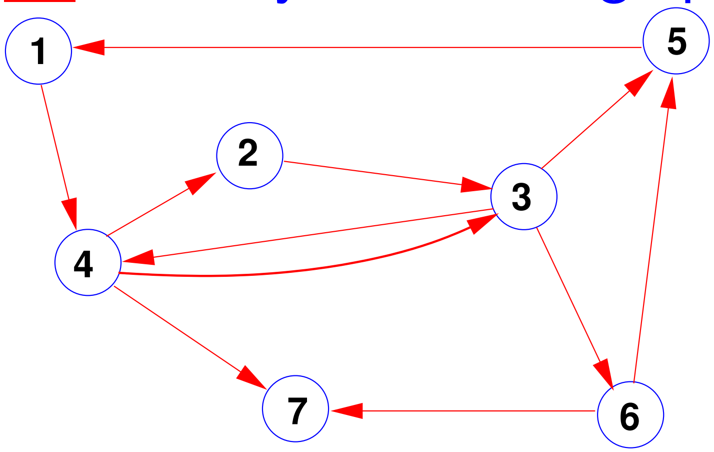
- A path is a sequence of vertices $w_0, w_1, \ldots, w_k$ such that $(w_i, w_{i+1}) \ \in E$ for $i = 0, \ldots, k-1$.

- The length of the path $w_0, w_1, \ldots, w_k$ is k (# of edges in the path)

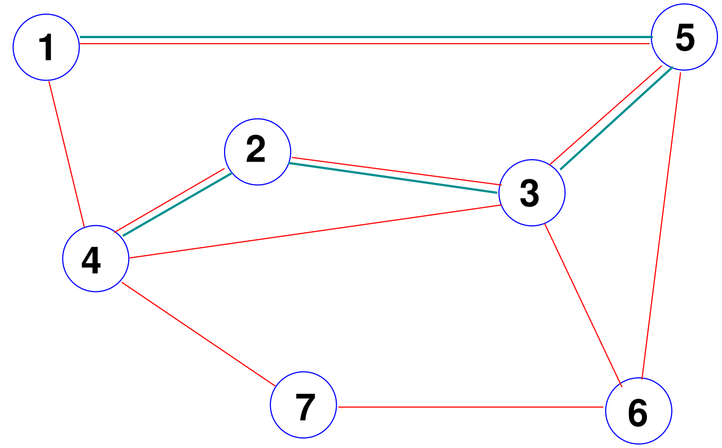
- A cycle is a closed path, i.e., a path with $w_k = w_0$.

- A graph is acyclic if it has no cycles.

Find cycles in this graph:



A path in an indirected graph



- A path $w_0, \ldots, w_k$ is simple if the vertices $w_0, \ldots, w_k$ are distinct (except that we may have $w_0 = w_k$ for cycles).

- An undirected graph is connected if there is path from every vertex to every other vertex.

- A digraph with the same property is said to be strongly connected

- The undirected form of a directed graph the undirected graph obtained by removing the directions of all the edges.

- Another term used "symmetrized" form -

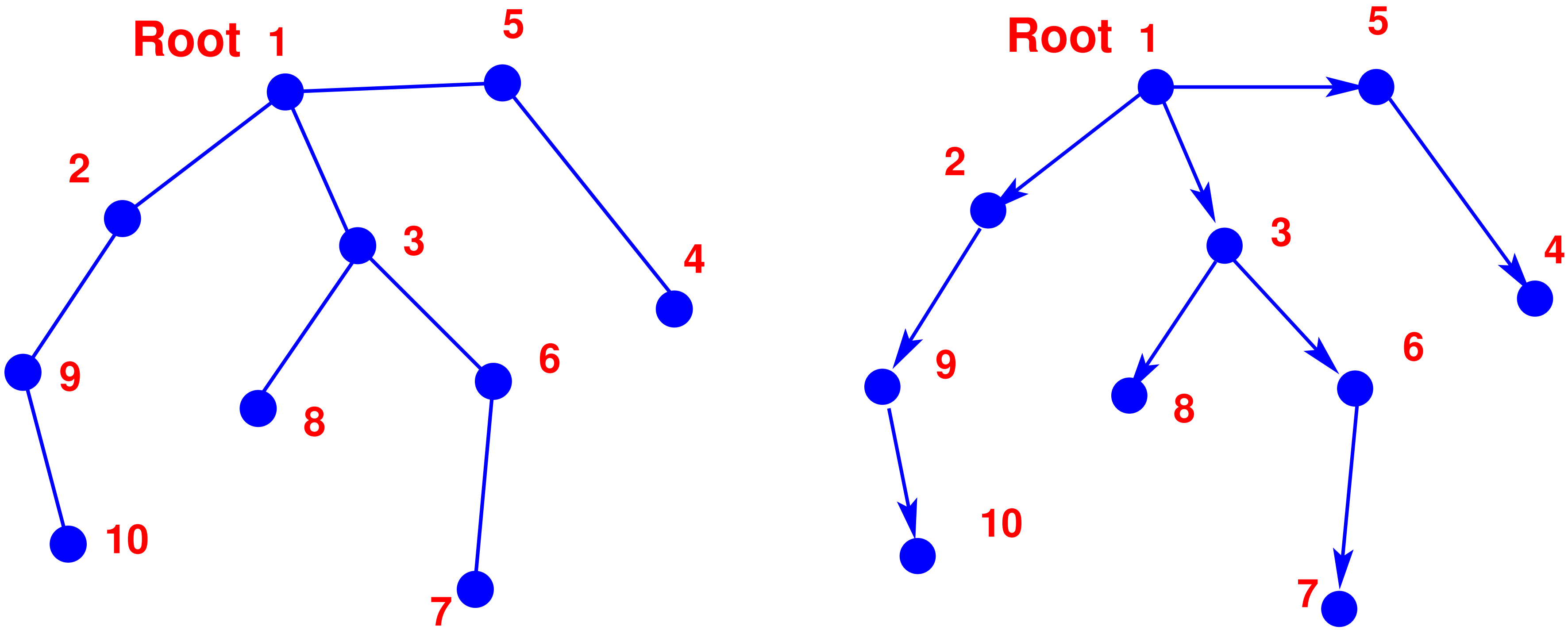
- A directed graph whose undirected form is connected is said to be weakly connected or connected.

- Tree = a graph whose undirected form, i.e., symmetrized form, is acyclic & connected

- Forest = a collection of trees

- In a rooted tree one specific vertex is designated as a root.

- Root determines orientation of the tree edges in parent-child relation



➤ Parent-Child relation: immediate neighbors of root are children. Root is their parent. Recursively define children-parents

➤ In example: v_3 is parent of v_6, v_8 and v_6, v_8 are chidren of v_3.

➤ Nodes that have no children are leaves. In example: v_{10}, v_7, v_8, v_4

➤ Descendent, ancestors, ...

Tree traversals

➤ Tree traversal is a process of visiting all vertices in a tree. Typically traversal starts at root.

➤ Want: systematic traversals of all nodes of tree – moving from a node to a child or parent

➤ Preorder traveral: Visit children before parent [recursively]

In example: $v_1, v_2, v_9, v_{10}, v_3, v_8, v_6, v_7, v_5, v_4$

➤ Preorder traveral: Visit parent then children [recursively]

In example : $v_{10}, v_9, v_2, v_8, v_7, v_6, v_3, v_4, v_5, v_1$

Graphs Traversals – Depth First Search

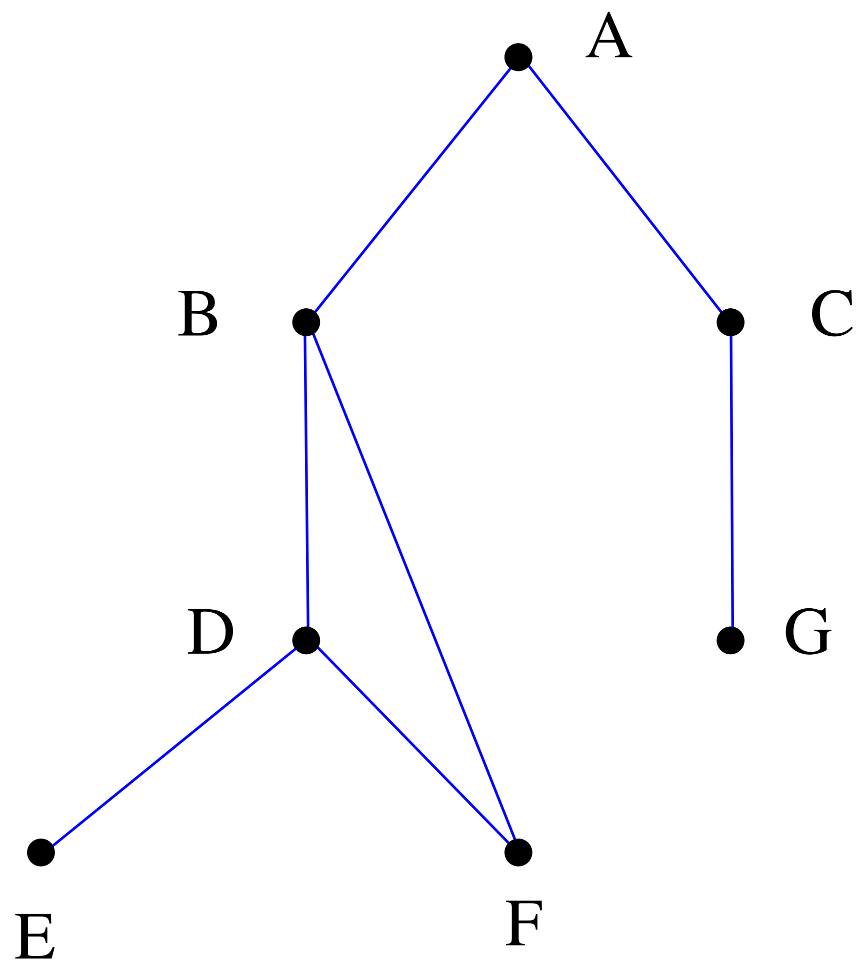
- Issue: systematic way of visiting all nodes of a general graph
- Two basic methods: Breadth First Search (to be seen later) and Depth-First Search
- Idea of DFS is recursive:

Algorithm $DFS(G, v)$ (DFS from v)

- Visit and Mark v;
- for all edges (v, w) do
  - if w is not marked then $DFS(G, w)$

- If G is undirected and connected, all nodes will be visited
- If G is directed and strongly connected, all nodes will be visited

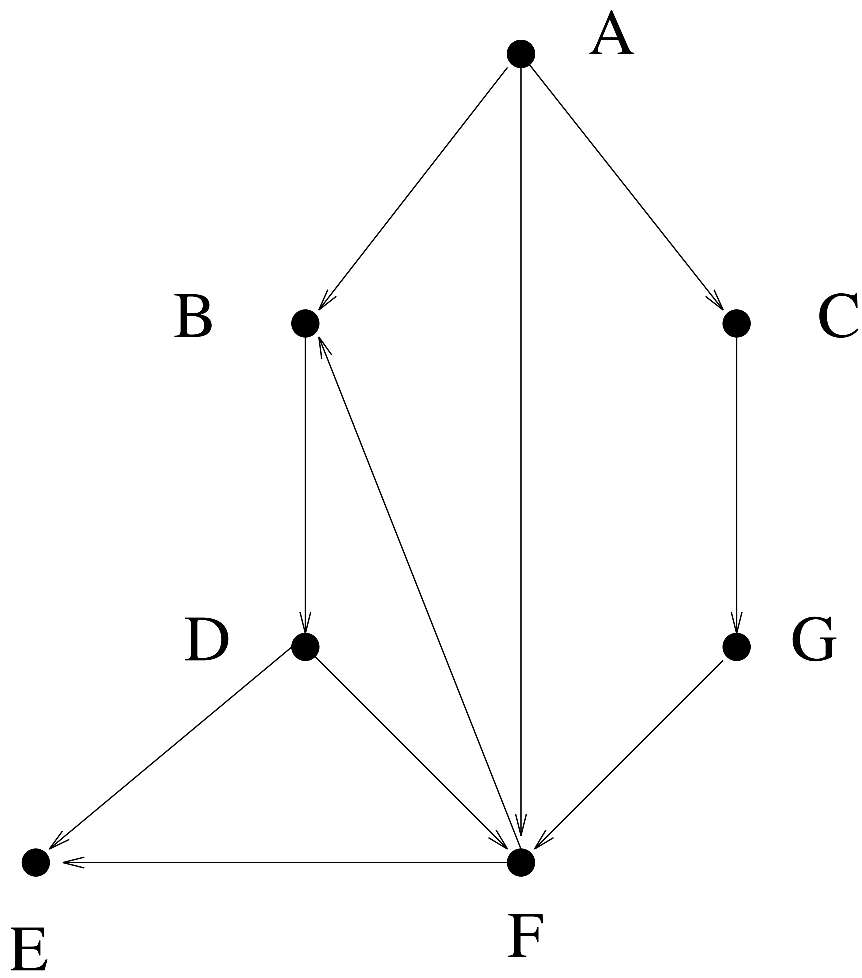
Depth First Search – undirected graph example



- Assume adjacent nodes are listed in alphabetical order.

DFS traversal from A: ?

Depth First Search – directed graph example



- Assume adjacent nodes are listed in alphabetical order.

DFS traversal from A: ?

Depth-First-Search Tree: Consider the parent-child relation: v is a parent of u if u was visited from v in the depth first search algorithm. The (directed) graph resulting from this binary relation is a tree called the Depth-First-Search Tree. To describe tree: only need the parents list.

➤ To traverse all the graph we need a DFS(v,G) from each node v that has not been visited yet – so add another loop. Refer to this as

$$\boxed{\text{DFS(G)}}$$

➤ When a new vertex is visited in DFS, some work is done. Example: we can build a stack of nodes visited to show order (reverse order: easier) in which the node is visited.

EXAMPLE

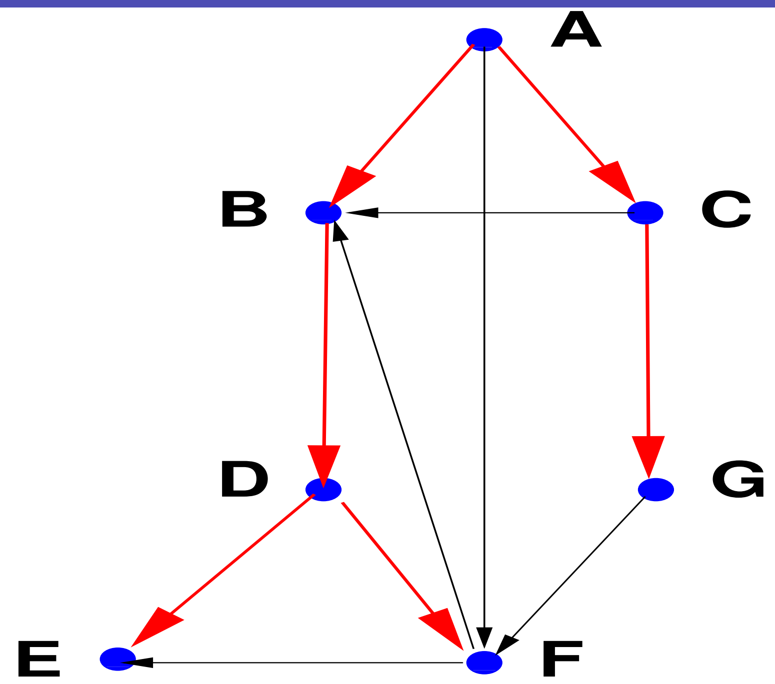
We assume adjacency list is in increasing order. [e.g: Adj(4)=(1,5,6,7)]

```
            3       5
            o       o
            |       |
            |       |
            |       |4      6
          1 o-------o-------o
           / \      |      /
          /   \     |     /
         /     \    |    /
        /       \   |   /
    2  o     7     o
```

```
DFS traversal: 1 --> 2 --> 3 --> 4  --> 5 --> 6 --> 7
Parents list:        1     1     1      4     4     6
```

```
        3   o       o 5
            |       |
            |       |4      6
          1 o-------o-------o        <-----  Depth First
           /               /                 Search Tree
          /               /
      2  o          7    o
```

Back edges, forward edges, and cross edges

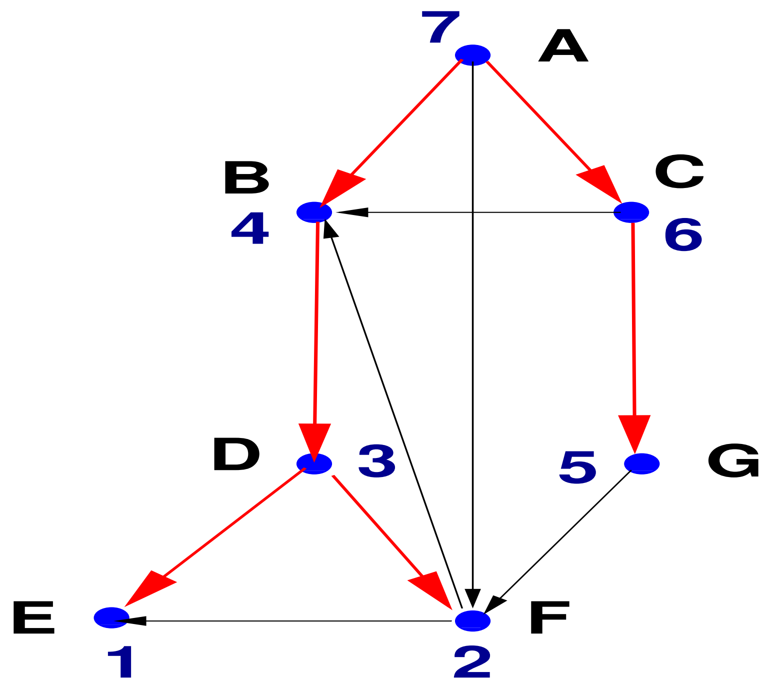


- Thick red lines: DFS traversal tree from A
- $A \rightarrow F$ is a Forward edge
- $F \rightarrow B$ is a Back edge
- $C \rightarrow B$ and $G \rightarrow F$ are Cross-edges.

Postorder traversal : label the nodes so that children in tree labeled before root.

➤ Important for some algorithms

➤ label(i) $==$ order of completion of visit of subtree rooted at node i



➤ Notice:

- Tree-edges / Forward edges : labels decrease in $\longrightarrow$
- Cross edges : labels decrease in $\longrightarrow$
- Back-edges : labels increase in $\longrightarrow$

Properties of Depth First Search

- If G is a connected undirected (or strongly directed) graph, then each vertex will be visited once and each edge will be inspected at least once.

- Therefore, for a connected undirected graph, The cost of DFS is $O(|V| + |E|)$

- If the graph is undirected, then there are no cross-edges. (all non-tree edges are called 'back-edges')

Theorem: A directed graph is acyclic iff a DFS search of G yields no back-edges.

Topological Sort

<u>The Problem:</u> Given a Directed Acyclic Graph (DAG), order the vertices from 1 to n such that, if (u, v) is an edge, then u appears before v in the ordering.

- Equivalently, label vertices from 1 to n so that in any (directed) path from a node labelled k, all vertices in the path have labels $> k$.
- Many Applications
- Prerequisite requirements in a program
- Scheduling of tasks for any project
- Parallel algorithms;
- ...

Topological Sorting: A first algorithm

Property exploited: An acyclic Digraph must have at least one vertex with indegree $= 0$.

✍ Prove this

Algorithm:

- First label these vertices as 1, 2, ..., k;
- Remove these vertices and all edges incident from them
- Resulting graph is again acyclic ... $\exists$ nodes with indegree $= \mathbf{0}$. label these nodes as $k+1, k+2, \ldots,$
- Repeat..

✍ Explore implementation aspects.

Alternative methods: Topological sort from DFS

- Depth first search traversal of graph.
- Do a 'post-order traversal' of the DFS tree.

<u>Algorithm $Lst = Tsort(G)$</u> (post-order DFS from v)

```
    Mark = zeros(n,1);   Lst = ∅
    for v=1:n do:
        if (Mark(v)== 0)
            [Lst, Mark] = dfs(v, G, Lst, Mark);
        end
    end
```

- dfs(v, G, Lst, Mark) is the DFS(G,v) which adds v to the top of Lst after finishing the traversal from v

Lst = DFS(G,v)

- Visit and Mark v;
- for all edges (v, w) do
  - if w is not marked then $Lst = DFS(G, w)$
- $Lst = [v, Lst]$

➤ Topological order given by the final Lst array of Tsort

✍ Explore implementation issue

✍ Implement in matlab

✍ Show correctness [i.e.: is this indeed a topol. order? hint: no back-edges in a DAG]

GRAPH MODELS FOR SPARSE MATRICES

- See Chap. 3 of text
- Sparse matrices and graphs.
- Bipartite model
- Graph Laplaceans. Application: Graph Partitioning

Graph Representations of Sparse Matrices. Recall:

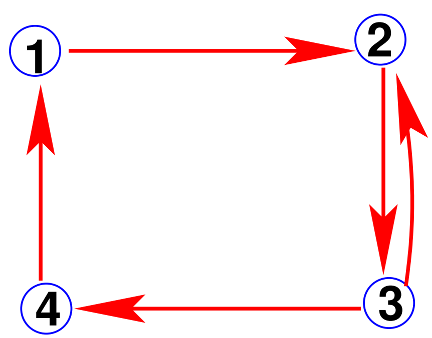
Adjacency Graph $G = (V, E)$ of an $n \times n$ matrix A :

$$V = \{1, 2, ..., N\} \qquad E = \{(i, j) | a_{ij} \neq 0\}$$

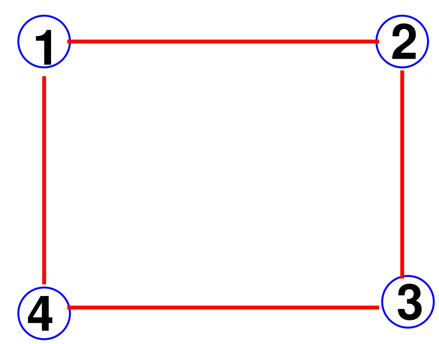
- G $==$ undirected if A has a symmetric pattern

Example:

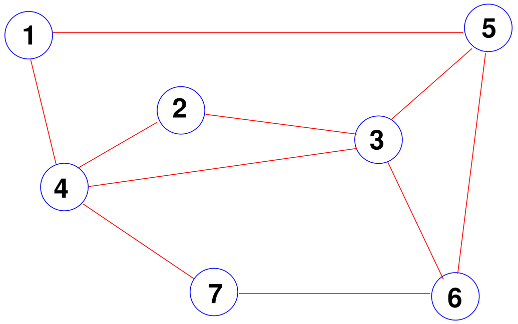
$$\begin{bmatrix} & \star & & \\ & & \star & \\ & \star & & \star \\ \star & & & \end{bmatrix}$$



$$\begin{bmatrix} & \star & & \star \\ \star & & \star & \\ & \star & & \star \\ \star & & \star & \end{bmatrix}$$



Show the matrix pattern for the graph on the right and give an interpretation of the path v_4, v_2, v_3, v_5, v_1 on the matrix



➤ A separator is a set Y of vertices such that the graph G_{X-Y} is disconnected.

Example: $Y = \{v_3, v_4, v_5\}$ is a separator in the above figure

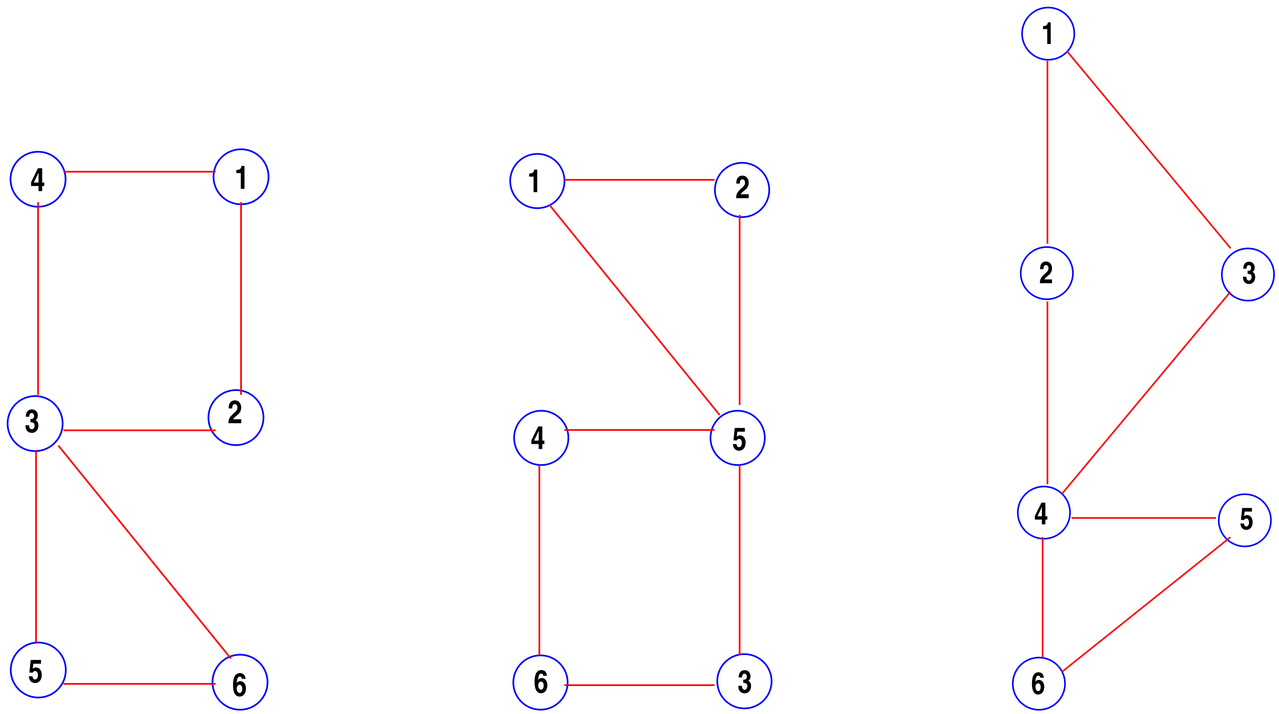
Example: Adjacency graph of:

$$A = \begin{bmatrix} & \star & & \star & & \\ \star & & \star & & & \\ & \star & & \star & \star & \star \\ \star & & \star & & & \\ & & \star & & & \star \\ & & \star & & \star & \end{bmatrix}.$$

Example: For any matrix A, what is the graph of A^2? [interpret in terms of paths in the graph of A]

➤ Two graphs are isomorphic is there is a mapping between the vertices of the two graphs that preserves adjacency.

✍ Are the following 3 graphs isomorphic? If yes find the mappings between them.



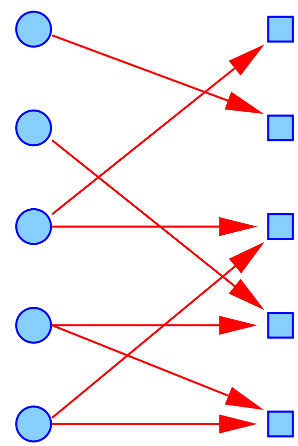
➤ Graphs are identical – labels are different

Bipartite graph representation

- Each row is represented by a vertex
- Each column is represented by a vertex
- Relations only between rows and columns.
- Row i is connected to column j if $a_{ij} \neq 0$

Example:

$$\begin{bmatrix} & \star & & & \\ & & & \star & \\ \star & & \star & & \\ & & & \star & \star \\ & & \star & & \star \end{bmatrix}$$



Interpretation of graphs of matrices

➤ Note: the bipartite model is used only for specific cases [e.g. rectangular matrices, ...] - By default we use the standard definition of graphs.

✍ What is the graph of $A + B$ (for two $n \times n$ matrices)?

✍ What is the graph of A^T ?

✍ What is the graph of $A.B$?

✍ What is the graph of A^k?

✍ In which of the following cases is the underlying physical mesh the same as the graph of $\boldsymbol{A}$ (in the sense that edges are the same):

- Finite difference mesh [consider the simple case of 5-pt and 7-pt FD problems - then 9-point meshes.]
- Finite element mesh with linear elements (e.g. triangles)?
- Finite element mesh with other types of elements? [to answer this question you would have to know more about higher order elements]

Graph Laplaceans - Definition

➤ "Laplace-type" matrices associated with general undirected graphs – useful in many applications

➤ Given a graph $G = (V, E)$ define

- A matrix W of weights w_{ij} for each edge
- Assume $w_{ij} \geq 0,$, $w_{ii} = 0$, and $w_{ij} = w_{ji}\ \forall(i, j)$
- The diagonal matrix $D = diag(d_i)$ with $d_i = \sum_{j \neq i} w_{ij}$

➤ Corresponding *graph Laplacean* of G is:

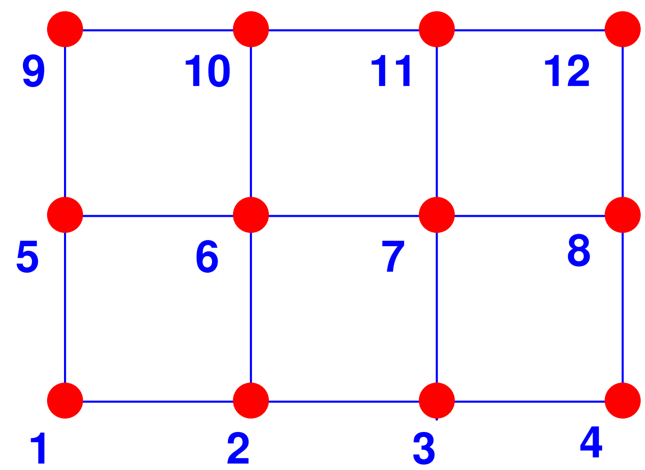
$$L = D - W$$

➤ Gershgorin's theorem $\rightarrow$ L is positive semidefinite

➤ Simplest case:

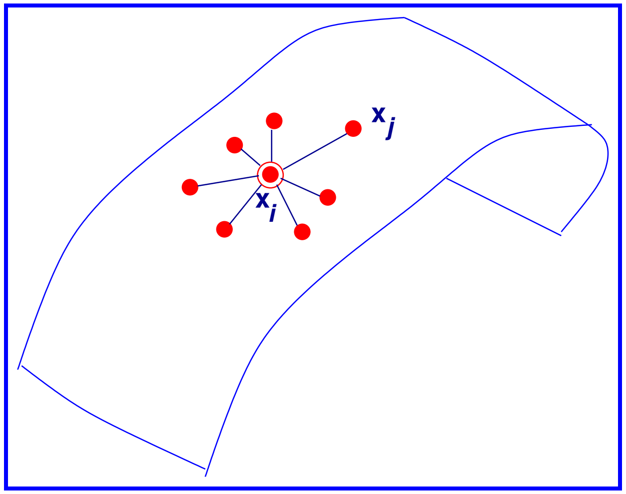
$$w_{ij} = \begin{cases} 1 \text{ if } (i,j) \in E \& i \neq j \\ 0 \quad \text{else} \end{cases} \qquad D = \text{diag}\left[d_i = \sum_{j \neq i} w_{ij}\right]$$

✍ Define the graph Laplacean for the graph associated with the simple mesh shown next. [use the simple weights of 0 or 1]



✍ What is the difference with the discretization of the Laplace operator in 2-D for case when mesh is the same as this graph?

A few properties of graph Laplaceans



Strong relation between $x^T L x$ and local distances between entries of x

➤ Let L = any matrix s.t. $L = D - W$, with $D = diag(d_i)$ and

$$w_{ij} \geq 0, \qquad d_i = \sum_{j \neq i} w_{ij}$$

Property 1: for any $x \in \mathbb{R}^n$:

$$x^\top L x = \frac{1}{2} \sum_{i,j} w_{ij} |x_i - x_j|^2$$

Property 2: (generalization) for any $\boldsymbol{Y} \in \mathbb{R}^{d \times n}$:

$$\mathrm{Tr}\left[\boldsymbol{Y}\boldsymbol{L}\boldsymbol{Y}^\top\right] = \frac{1}{2}\sum_{i,j} w_{ij}\|\boldsymbol{y}_i - \boldsymbol{y}_j\|^2$$

Property 3: For the particular $\boldsymbol{L} = \boldsymbol{I} - \frac{1}{n}\boldsymbol{1}\boldsymbol{1}^\top$

$$\boldsymbol{X}\boldsymbol{L}\boldsymbol{X}^\top = \bar{\boldsymbol{X}}\bar{\boldsymbol{X}}^\top == n \times \text{Covariance matrix}$$

Property 4: $\boldsymbol{L}$ is singular and admits the null vector $\boldsymbol{e}$ =`ones(n,1)`

Property 5: (Graph partitioning) Consider situation when $w_{ij} \in \{0, 1\}$. If x is a vector of signs (± 1) then

$$x^\top L x = 4 \times (\text{'number of edge cuts'})$$

edge-cut = pair (i, j) with $x_i \neq x_j$

➤ Would like to minimize (Lx, x) subject to $x \in \{-1, 1\}^n$ and $e^T x = 0$ [balanced sets]

➤ WIl solve a relaxed form of this problem

- Consider any symmetric (real) matrix A with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ and eigenvectors $u_1, \cdots, u_n$

- Recall that:
(Min reached for $x = u_1$)

$$\min_{x \in \mathbb{R}^n} \frac{(Ax, x)}{(x, x)} = \lambda_1$$

- In addition:
(Min reached for $x = u_2$)

$$\min_{x \perp u_1} \frac{(Ax, x)}{(x, x)} = \lambda_2$$

- For a graph Laplacean $u_1 = e =$ vector of all ones and

- ...vector u_2 is called the Fiedler vector. It solves a relaxed form of the problem -

$$\min_{x \in \{-1,1\}^n;\ e^T x = 0} \frac{(Lx, x)}{(x, x)} \quad \rightarrow \quad \min_{x \in \mathbb{R}^n;\ e^T x = 0} \frac{(Lx, x)}{(x, x)}$$

- Define $v = u_2$ then $lab = sign(v - med(v))$