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.

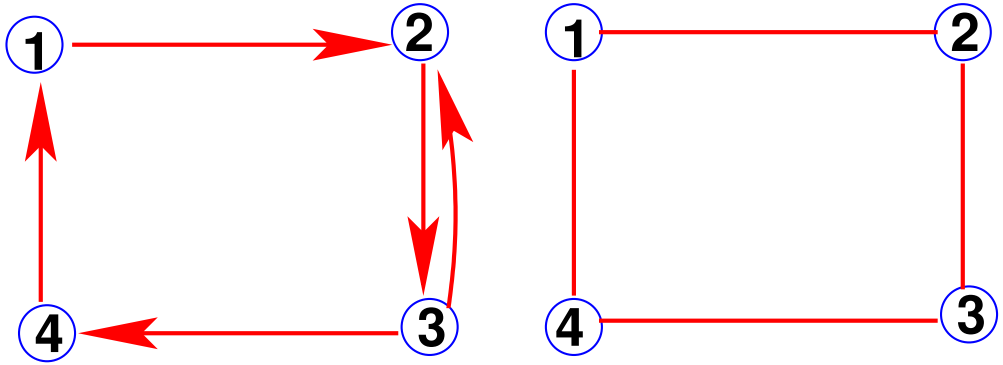
If R is a binary relation between elements in V then, we can represent it by a graph $G = (V, E)$ as follows:

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

Undirected graph $\leftrightarrow$ symmetric relation

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

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



✍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)]

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

Graphs – Examples and applications

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. Social Networks;
7. Sparse matrices;

...

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

➤ $Adj(i) = \{j | j$ 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 $i \to i$ 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.

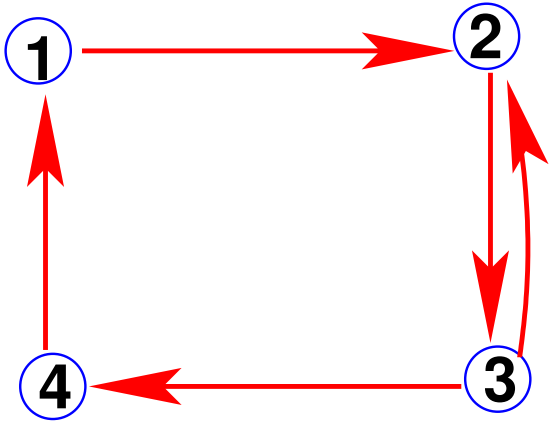
Adjacency matrix Assume $V = \{1, 2, \cdots, n\}$. Then the adjacency matrix of $G = (V, E)$ is the $n \times n$ matrix, with entries:

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

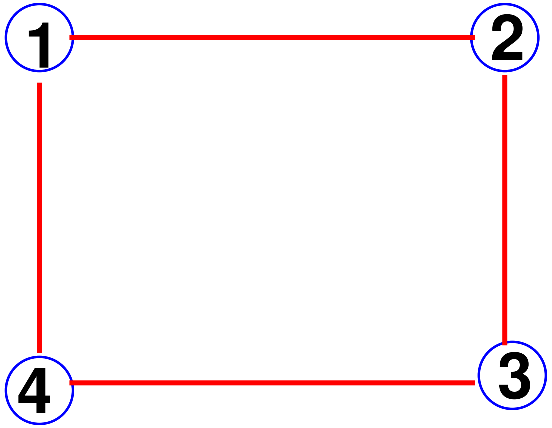
Representations of Graphs (cont.)

Example:

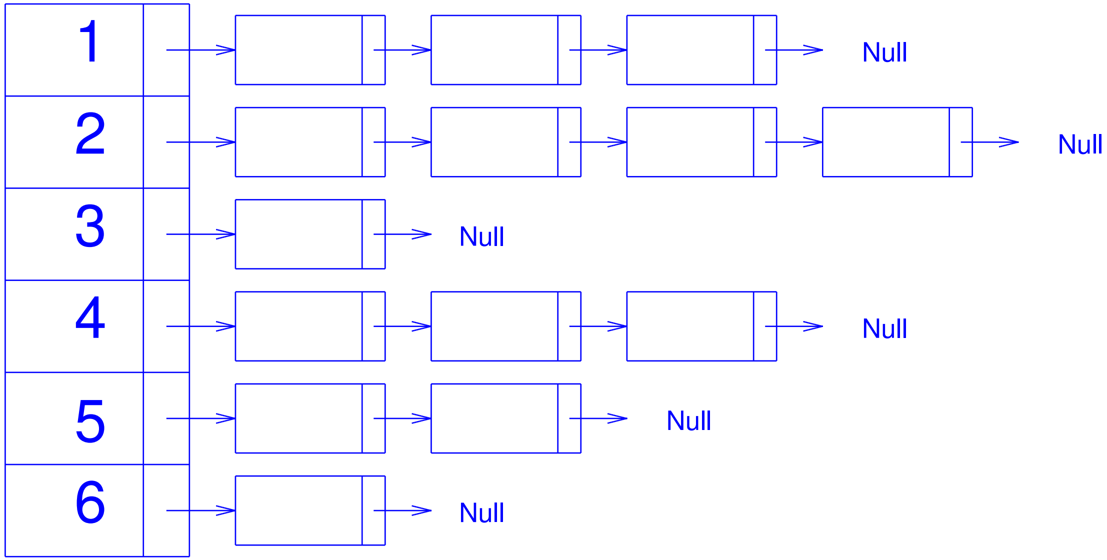
$$\begin{bmatrix} & 1 & & \\ & & 1 & \\ & 1 & & 1 \\ 1 & & & \end{bmatrix}$$



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



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) - but not 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 ($\rightarrow$ dense block in matrix)

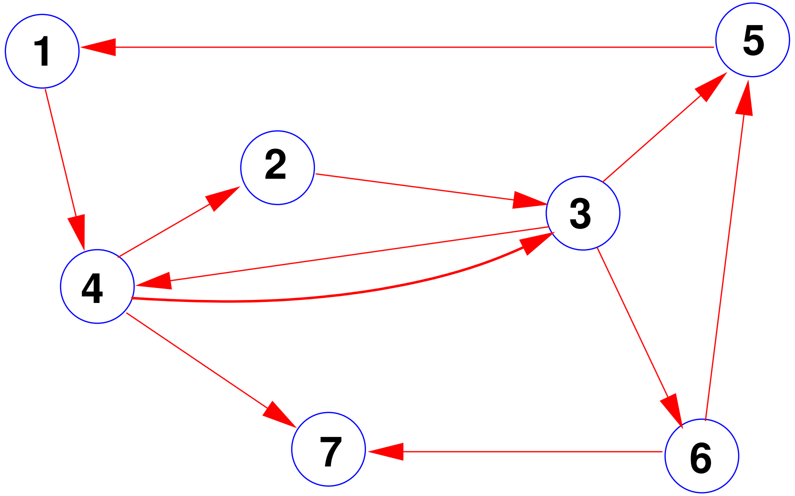
- A path is a sequence of vertices $w_0, w_1, \ldots, w_k$ such that $(w_i, w_{i+1}) \in E$ for $i = 0, \ldots, k-1$.

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

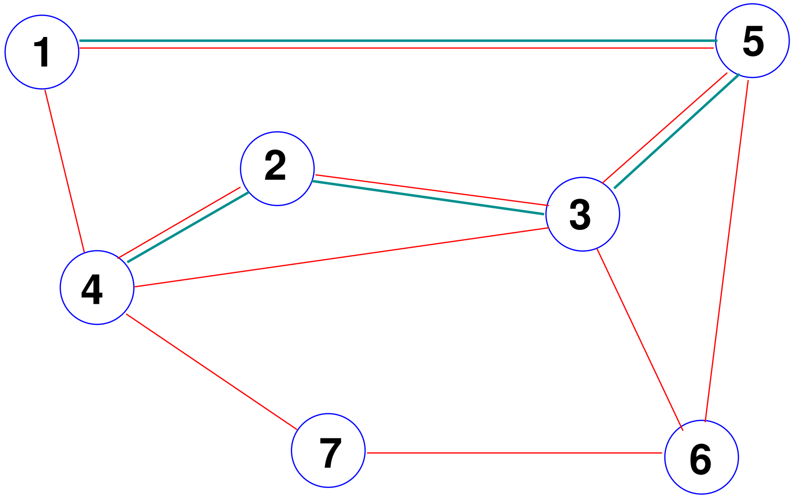
- A cycle is a closed path, i.e., a path with $w_k = w_0$.

- A graph is acyclic if it has no cycles.

✍2 Find cycles in this graph:

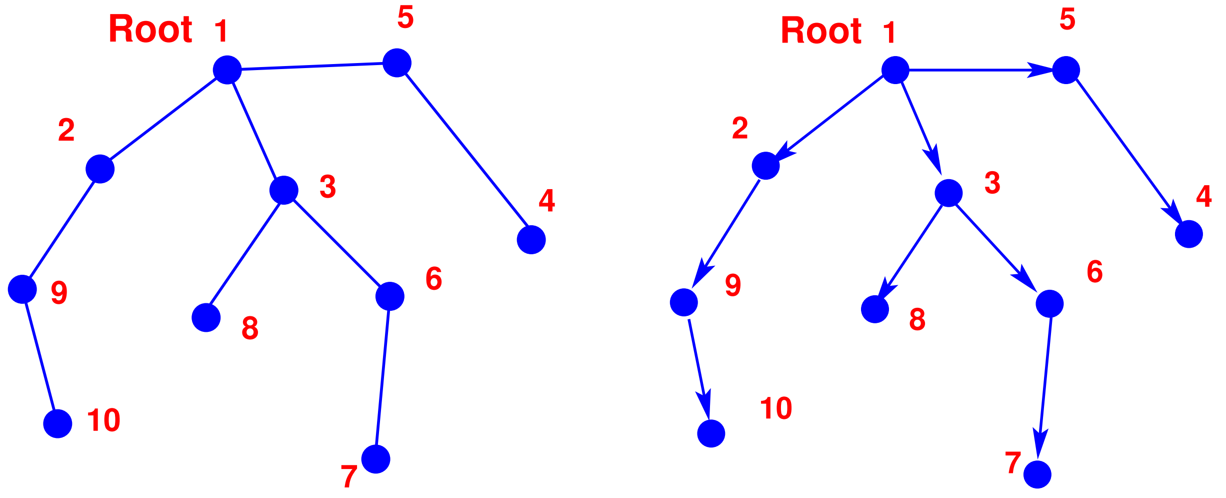


A path in an indirected graph



- 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 <u>directed</u> 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 traversal: Visit parent before children [recursively]

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

➤ Postorder traversal: Visit children before parent [recursively]

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

Graph Traversals – Depth First Search

- Issue: systematic way of visiting all nodes of a general graph
- Two basic methods: Breadth First Search (wll's see later) & ...
- Depth-First Search

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

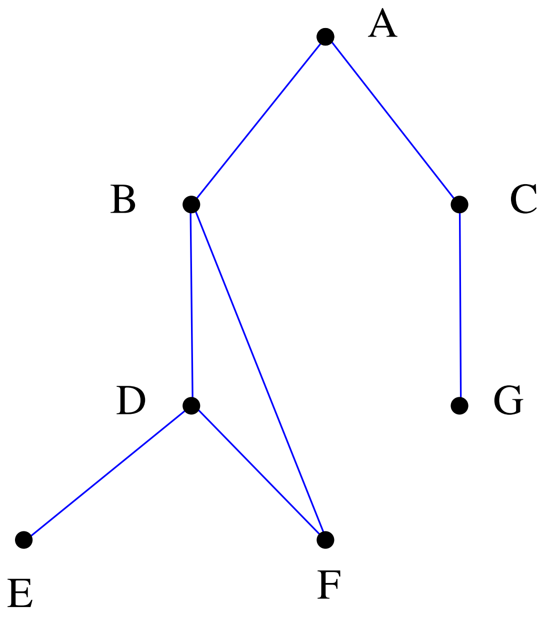
  - Visit and Mark v;
  - for all edges (v, w) do
    - if w is not marked then $List = DFS(G, w)$
    - Add v to top of list produced above

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

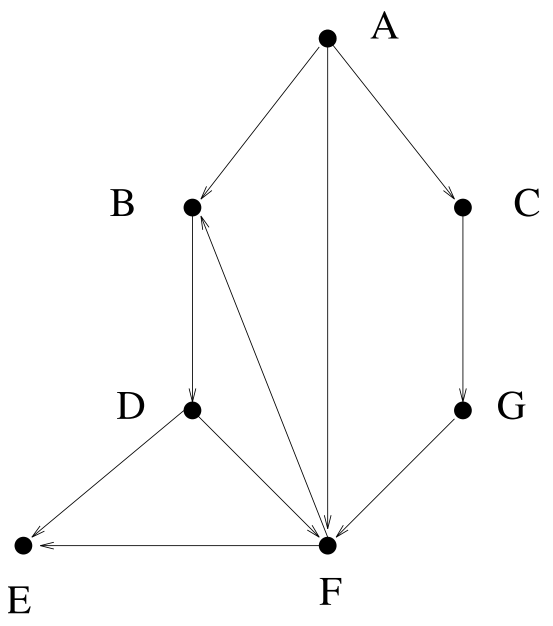
Depth First Search – undirected graph example

➤ Assume adjacent nodes are listed in alphabetical order.

✍3 DFS traversal from A ?



Depth First Search – directed graph example



➤ Assume adjacent nodes are listed in alphabetical order.

✍4 DFS traversal from A?

NOTE: We will now use a column-oriented graph representation:

$$j \rightarrow i \quad \text{if} \quad a_{ij} \neq 0$$

```
    function [Lst, Mark] = dfs(u, A, Lst, Mark)
%% function [Lst, Mark] = dfs(u, A, Lst, Mark)
%% dfs from node u  -- Recursive
%%-----------------------------------
[ii, jj, rr] = find(A(:,u));
Mark(u) = 1;
for k=1:length(ii)
     v = ii(k);
     if (~Mark(v))
         [Lst, Mark] = dfs(v, A, Lst, Mark);
     end
end
Lst = [u,Lst]
```

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

DFS(G)

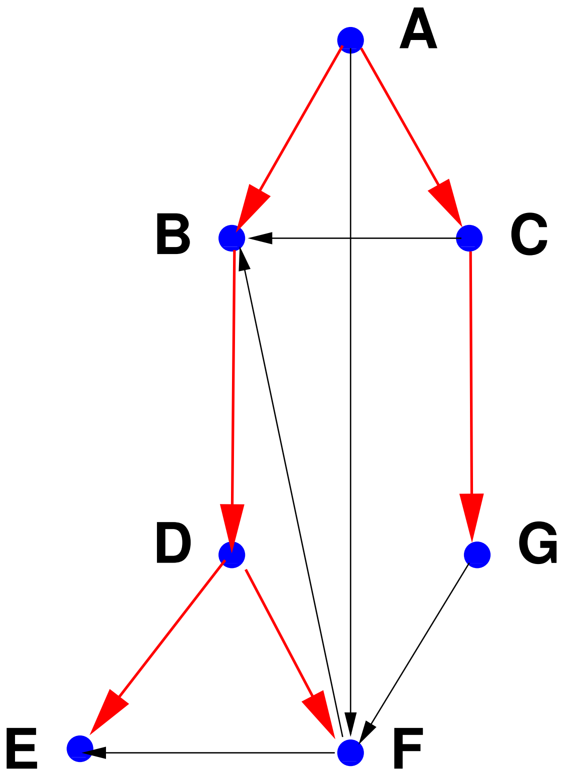
- When a new vertex is visited in DFS, some work is done. Example: we can build a stack of nodes visited to show order (reverse order: easier) in which the node is visited.

```
EXAMPLE       3     5      We assume adjacency list
              o     o      is in increasing order.
              |     |      [e.g: Adj(4)=(1,5,6,7)]
              |     |
              |     |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



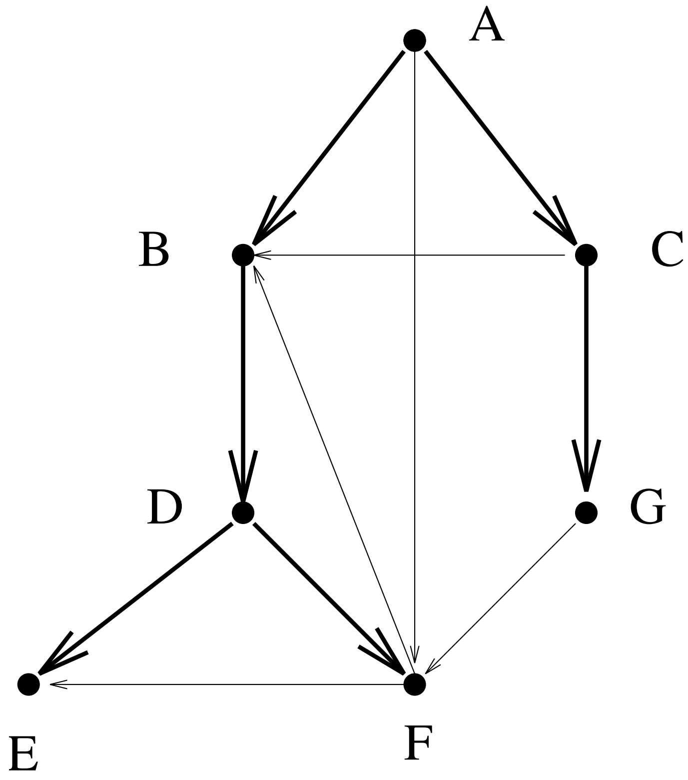
- Thick red lines: DFS traversal tree from A
- $A \rightarrow F$ is a Forward edge
- $F \rightarrow B$ is a Back edge
- $C \rightarrow B$ and $G \rightarrow F$ are Cross-edges.

➤ Consider the 'List' produced by DFS.

`Lst=[A, C, G, B, D, F, E]`

➤ Order in list is important for some algorithms

➤ Notice: Label nodes in List from 1 to n . Then:



- Tree-edges / Forward edges : labels increase in $\rightarrow$
- Cross edges : labels in/de-crease in $\rightarrow$ [depends on labeling]
- Back-edges : labels decrease in $\rightarrow$

Properties of Depth First Search

- If G is a connected undirected (or strongly connected) 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.

- Terminology: Directed Acyclic Graph or *DAG*

Topological Sort

Problem: 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.

✍5 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 ... ∃ nodes with indegree $= 0$. label these nodes as $k+1, k+2, \ldots,$
- Repeat..

✍6 Explore implementation aspects.

Alternative method: Topological sort from DFS

➤ Depth first search traversal of graph.

➤ Do a 'post-order traversal' of the DFS tree.

Algorithm $Lst = Tsort(G)$

```
(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

✍7 Explore implementation issue

✍8 Implement in matlab

✍9 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, hypergraphs*
- *Application: back propagation*

Graph Representations of Sparse Matrices. Recall:

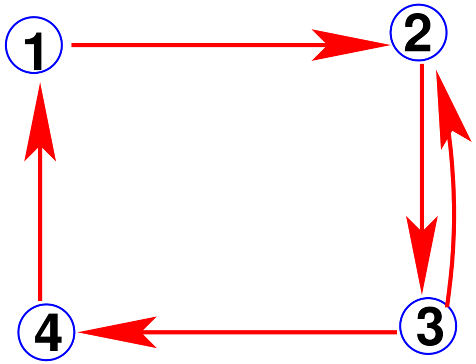
Adjacency Graph $G = (V, E)$ of an $n \times n$ matrix A :

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

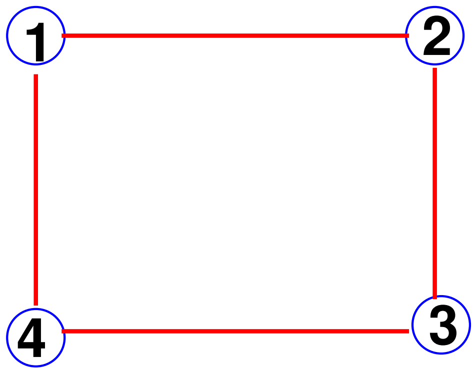
➤ G == undirected if A has a symmetric pattern

Example:

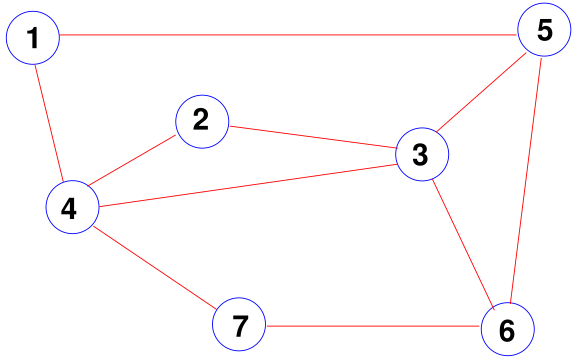
$$\begin{bmatrix} & \star & & \\ & & \star & \\ & \star & & \star \\ \star & & & \end{bmatrix}$$



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



✍10 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

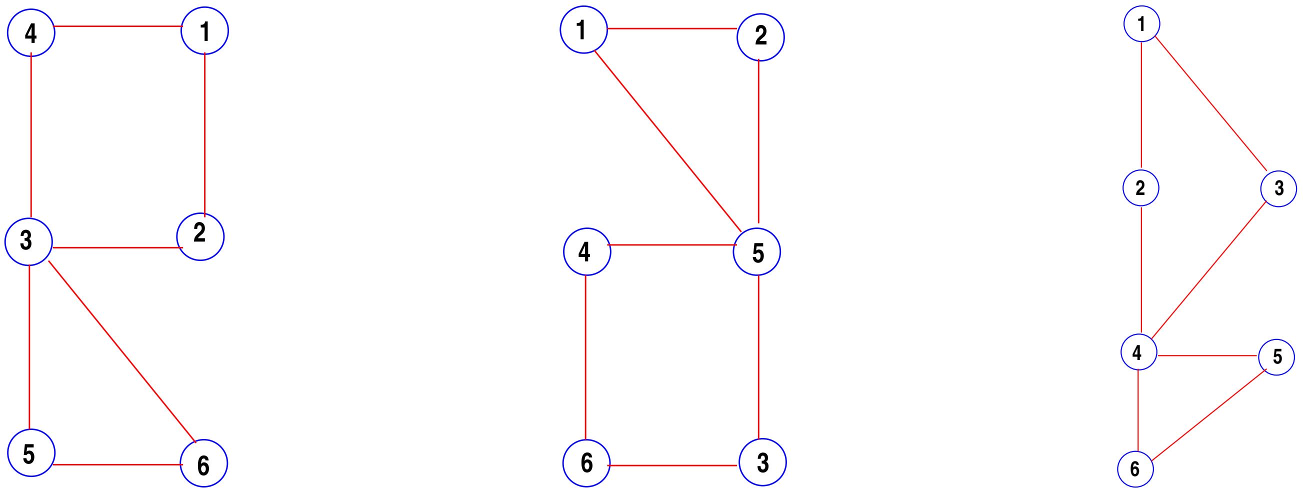
Example: Adjacency graph of:

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

Example: For any adjacency 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.

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



➤ Graphs are identical – labels are different

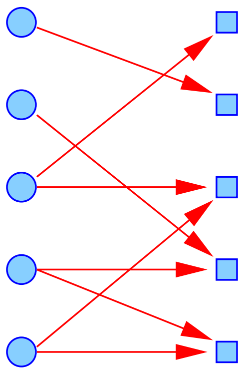
➤ Determinig graph isomorphism is a hard problem

Bipartite graph representation

- Rows and columns are (both) represented by vertices;
- Relations only between rows and columns: Row i is connected to column j if $a_{ij} \neq 0$

Example:

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



- Bipartite models used only for specific cases [e.g. rectangular matrices, ...] - By default we use the standard definition of graphs.

Interpretation of graphs of matrices

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

✍13 What is the graph of A^T ?

✍14 What is the graph of $A.B$?

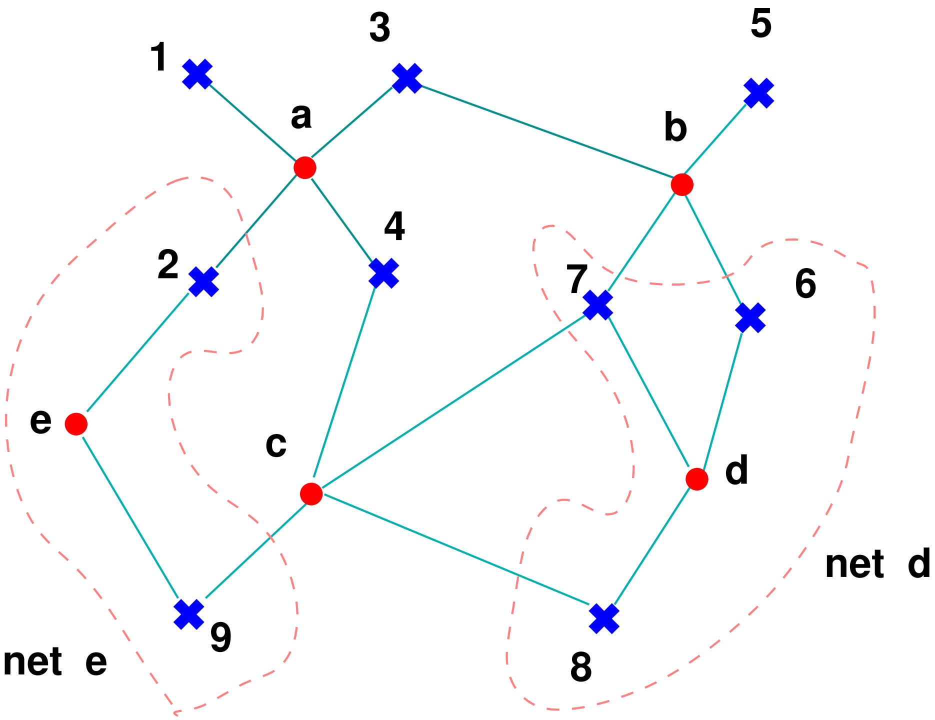
A few words on hypergraphs

- Hypergraphs are very general.. Ideas borrowed from VLSI work
- Main motivation: to better represent communication volumes when partitioning a graph. Standard models face many limitations
- Hypergraphs can better express complex graph partitioning problems and provide better solutions.
- Example: completely nonsymmetric patterns ...
- .. Even rectangular matrices. Best illustration: Hypergraphs are ideal for text data

Example: $V = \{1, \ldots, 9\}$ and $E = \{a, \ldots, e\}$ with

$a = \{1, 2, 3, 4\}$, $b = \{3, 5, 6, 7\}$, $c = \{4, 7, 8, 9\}$,

$d = \{6, 7, 8\}$, and $e = \{2, 9\}$

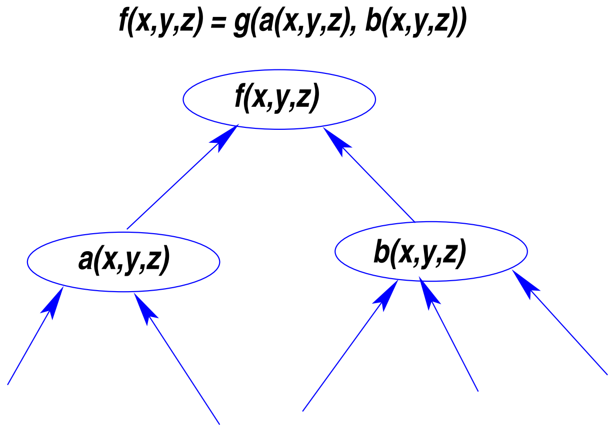


Boolean matrix:

$$A = \begin{array}{c} \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \end{matrix} \\ \boxed{\begin{matrix} 1 & 1 & 1 & 1 & & & & & \\ & & 1 & & 1 & 1 & 1 & & \\ & & & 1 & & & 1 & 1 & 1 \\ & & & & & 1 & 1 & 1 & \\ & 1 & & & & & & & 1 \end{matrix}} \end{array} \begin{matrix} \\ a \\ b \\ c \\ d \\ e \end{matrix}$$

A few words on computational graphs

➤ Computational graphs: graphs where nodes represent computations whose evaluation depend on other (incoming) nodes.



➤ Consider the following expression:

$$g(x, y) = (x + y - 2) * (y + 1)$$

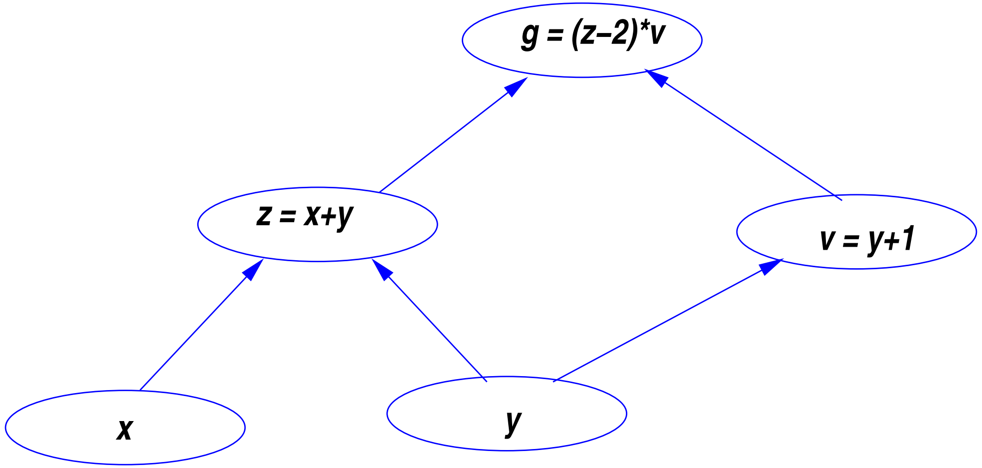
We can decompose this as
$$\begin{cases} z = x + y \\ v = y + 1 \\ g = (z - 2) * v \end{cases}$$

➤ Computational graph $\rightarrow$

➤ Given x, y we want:

(a) Evaluate the nodes and

(b) derivatives w.r.t x, y



(a) is trivial - just follow the graph up - starting from the leaves (that contain x and y)

(b): Use the chain rule – here shown for x only using previous setting

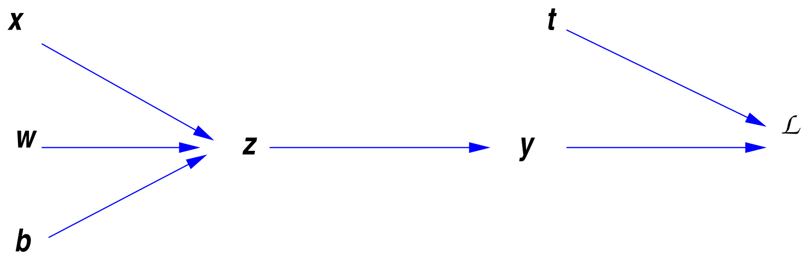
$$\frac{\partial g}{\partial x} = \frac{\partial g}{\partial a}\frac{da}{dx} + \frac{\partial g}{\partial b}\frac{db}{dx}$$

✍15 For the above example compute values and derivatives at all nodes when $x = -1, y = 2$.

Back-Propagation

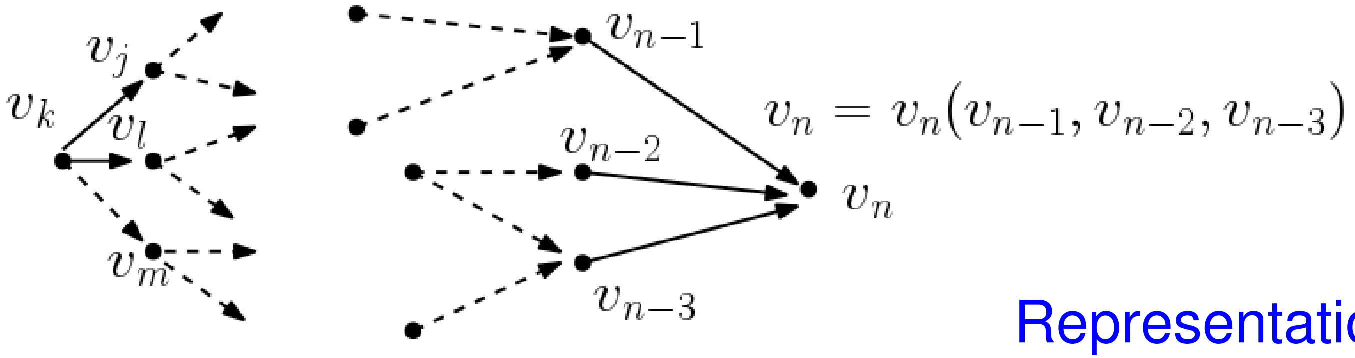
- Often we want to compute the gradient of the function at the root, once the nodes have been evaluated
- The derivatives can be calculated by going backward (or down the tree)
- Here is a very simple example from Neural Networks

$$\begin{cases} L = \frac{1}{2}(y-t)^2 \\ y = \sigma(z) \\ z = wx + b \end{cases}$$



- Note that t (desired output) and x (input) are constant.

Back-Propagation: General computational graphs



Representation: *a DAG*

- Last node (v_n) is the target function. Let us rename it f.
- Nodes $v_i, i = 1, \cdots, e$ with indegree 0 are the variables
- Want to compute $\partial f/\partial v_1, \partial f/\partial v_2, \cdots, \partial f/\partial v_e$
- Use the chain rule. $\longrightarrow$

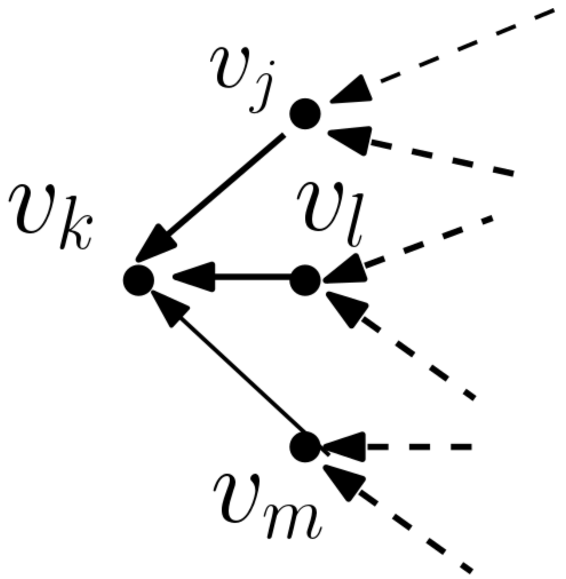
$$\frac{\partial f}{\partial v_k} = \frac{\partial f}{\partial v_j}\frac{\partial v_j}{\partial v_k} + \frac{\partial f}{\partial v_l}\frac{\partial v_l}{\partial v_k} + \frac{\partial f}{\partial v_m}\frac{\partial v_m}{\partial v_k}$$

➤ Let $\delta_k = \frac{\partial f}{\partial v_k}$ (called 'errors'). Then

$$\delta_k = \delta_j \frac{\partial v_j}{\partial v_k} + \delta_l \frac{\partial v_l}{\partial v_k} + \delta_m \frac{\partial v_m}{\partial v_k}$$

➤ To compute the δ_k's once the v_j's have been computed (in a 'forward' propagation) – proceed backward.

➤ $\delta_j, \delta_l, \delta_m$ available and $\partial v_i / \partial v_k$ computable. Nore $\delta_n \equiv 1$.



➤ However: cannot just do this in any order. Must follow a topological order in order to obey dependencies.

Example: