BACKGROUND: A Brief Introduction to Graph Theory

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

Graphs – definitions & representations

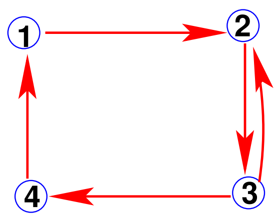
➤ Graph theory is a fundamental tool in sparse matrix techniques.

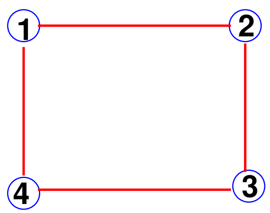
DEFINITION. A graph G is defined as a pair of sets $G = (V, E)$ with $E \subset V \times V$. So G represents a binary relation. The graph is undirected if the binary relation is symmetric. It is directed otherwise. V is the vertex set and E is the edge set.

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)

✍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

➤ 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. 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.

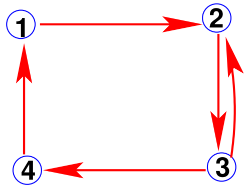
Adjacency matrix Assume $V = \{1, 2, \cdots, n\}$. Then the adjacency matrix of $G = (V, E)$ is the $n \times n$ matrix, with entries:

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

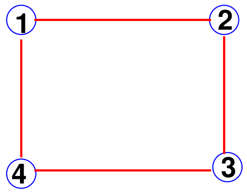
Representations of Graphs (cont.)

Example:

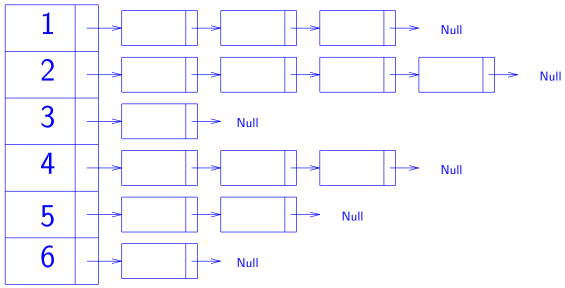
$$\begin{bmatrix} & 1 & & \\ & & 1 & \\ & 1 & & 1 \\ 1 & & & \end{bmatrix}$$



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



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).

➤ 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 ($\rightarrow$ dense block in matrix)

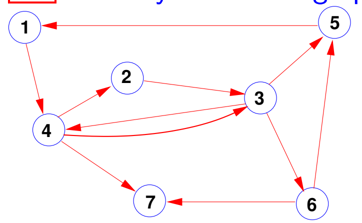
➤ A path is a sequence of vertices $w_0, w_1, \ldots, w_k$ such that $(w_i, w_{i+1}) \in E$ for $i = 0, \ldots, k-1$.

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

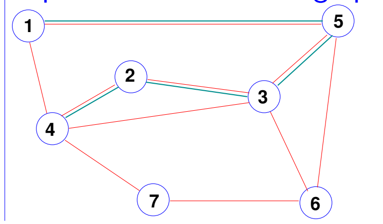
➤ A cycle is a closed path, i.e., a path with $w_k = w_0$.

➤ 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 -

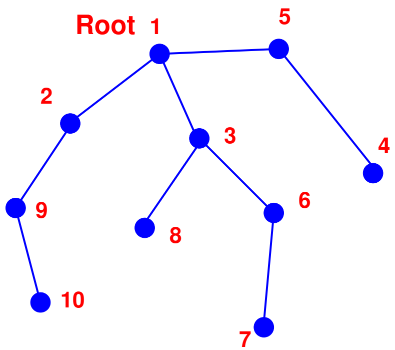
➤ A <u>directed</u> graph whose undirected form is connected is said to be weakly connected or connected.

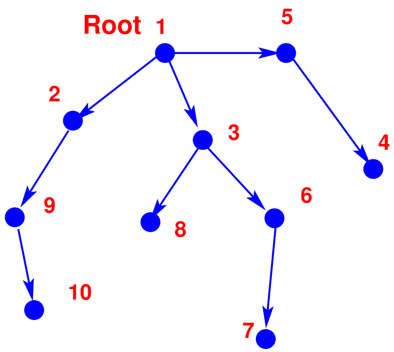
➤ Tree = a graph whose undirected form, i.e., symmetrized form, is acyclic & connected

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

Graphs 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

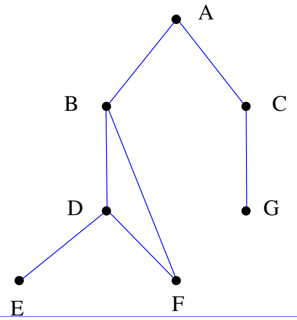
➤ If G is undirected and connected, all nodes will be visited

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

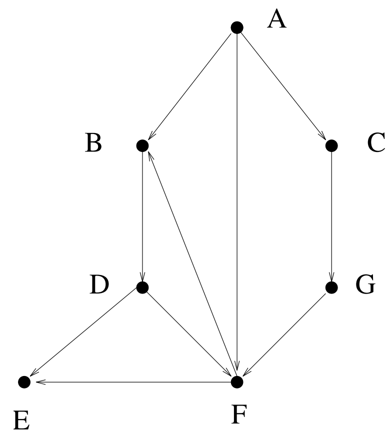
Depth First Search – undirected graph example

➤ 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?

```
  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.

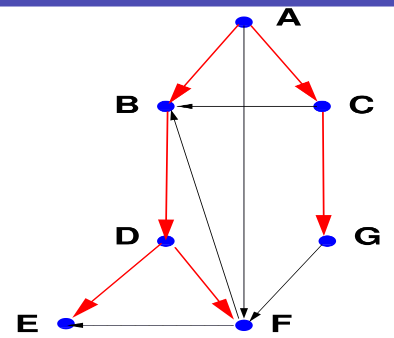
- To traverse all the graph we need a DFS(v,G) from each node v that has not been visited yet – so add another loop. Refer to this as

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

- 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        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

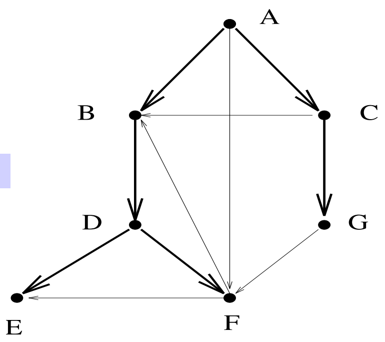


- Thick red lines: DFS traversal tree from A
- $A \rightarrow F$ is a Forward edge
- $F \rightarrow B$ is a Back edge
- $C \rightarrow B$ and $G \rightarrow F$ are Cross-edges.

➤ 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 $\longrightarrow$
- Cross edges : labels in/de-crease in $\longrightarrow$ [depends on labeling]
- Back-edges : labels decrease in $\longrightarrow$

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

The 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 methods: 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: Paths in graphs, Markov chains**

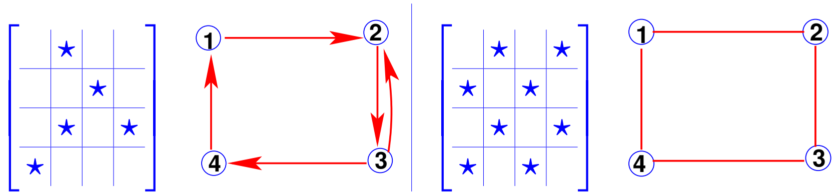
Graph Representations of Sparse Matrices. Recall:

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

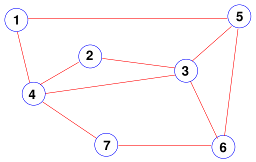
$$V = \{1, 2, ..., N\} \qquad E = \{(i, j) | a_{ij} \neq 0\}$$

➤ G == undirected if A has a symmetric pattern

Example:



✍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

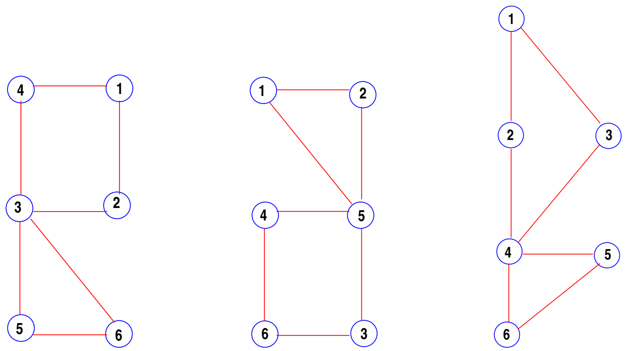
Example: Adjacency graph of:

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

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

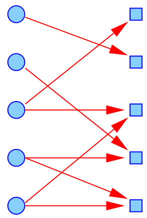
Bipartite graph representation

➤ 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:

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



➤ 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 In which of the following cases is the underlying physical mesh the same as the graph of 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]

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

✍14 What is the graph of A^T ?

✍15 What is the graph of $A.B$?

Paths in graphs

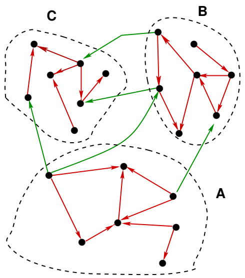
✍16 What is the graph of A^k?

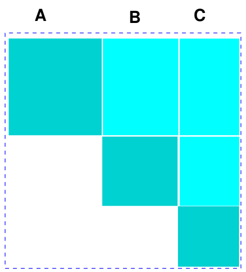
Theorem Let A be the adjacency matrix of a graph $G = (V, E)$. Then for $k \geq 0$ and vertices u and v of G, the number of paths of length k starting at u and ending at v is equal to $(A^k)_{u,v}$.

Proof: Proof is by induction. ■

➤ Recall (definition): A matrix is *reducible* if it can be permuted into a block upper triangular matrix.

➤ Note: A matrix is reducible iff its adjacency graph is not (strongly) connected, i.e., iff it has more than one connected component.





➤ No edges from C to A or B. No edges from B to A.

Theorem: Perron-Frobenius An irreducible, nonnegative $n \times n$ matrix A has a real, positive eigenvalue λ_1 such that:
(i) λ_1 is a simple eigenvalue of A;
(ii) λ_1 admits a positive eigenvector u_1 ; and
(iii)$|\lambda_i| \leq \lambda_1$ for all other eigenvalues λ_i where $i > 1$.

➤ The spectral radius is equal to the eigenvalue λ_1

➤ Definition : a graph is d regular if each vertex has the same degree d.

Proposition: The spectral radius of a d regular graph is equal to d.

Proof: The vector e of all ones is an eigenvector of A associated with the eigenvalue $\lambda = d$. In addition this eigenvalue is the largest possible (consider the infinity norm of A). Therefore e is the Perron-Frobenius vector u_1. ■

Application: Markov Chains

- Read about Markov Chains in Sect. 10.9 of: https://www-users.cs.umn.edu/~saad/eig_book_2ndEd.pdf
- The stationary probability satisfies the equation:

$$\boxed{\pi P = \pi}$$

Where π is a row vector.

- P is the probabilty transition matrix and it is 'stochastic':

A matrix P is said to be *stochastic* if :
(i) $p_{ij} \geq 0$ for all i, j
(ii) $\sum_{j=1}^{n} p_{ij} = 1$ for $i = 1, \cdots, n$
(iii) No column of P is a zero column.

- Spectral radius is ≤ 1 [Why?]
- Assume P is irreducible. Then:
- Perron Frobenius $\rightarrow \rho(P) = 1$ is an eigenvalue and associated eigenvector has positive entries.
- Probabilities are obtained by scaling π by its sum.
- Example: One of the 2 models used for page rank.

Example: A college Fraternity has 50 students at various stages of college (Freshman, Sophomore, Junior, Senior). There are 6 potential stages for the following year: Freshman, Sophomore, Junior, Senior, graduated, or left-without degree. Following table gives probability of transitions from one stage to next

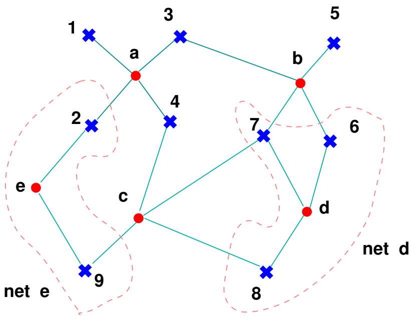
To \ From	Fr	So.	Ju.	Sr.	Grad	lwd
Fr.	.2	0	0	0	0	0
So.	.6	.1	0	0	0	0
Ju.	0	.7	.1	0	0	0
Sr.	0	0	.8	.1	0	0
Grad	0	0	0	.75	1	0
lwd	.2	.2	.1	.15	0	1

✍17 What is P? Assume initial population is $x_0 = [10, 16, 12, 12, 0, 0]$ and do a follow the population for a few years. What is the probability that a student will graduate? What is the probability that s/he leaves without a degree?

A few words about 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 $e = \{2, 9\}$



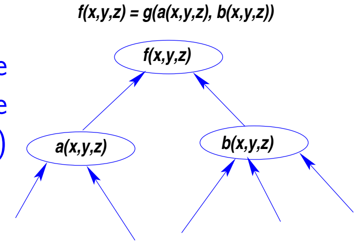
Boolean matrix:

$A =$

	1	2	3	4	5	6	7	8	9
a	1	1	1	1					
b			1		1	1	1		
c				1			1	1	1
d						1	1	1	
e		1							1

A few words on computational graphs

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

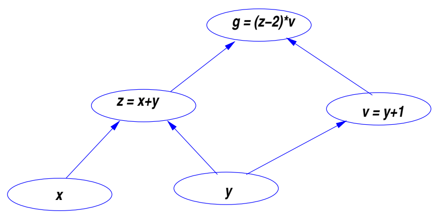


➤ Consider the following expression:

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

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

➤ Corresponding computational graph:



➤ Given values of x, y we want to (a) Evaluate the nodes and also (b) derivatives of g w.r.t x, y at the nodes

(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

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

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

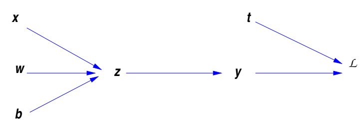
Back-Propagation

➤ 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)

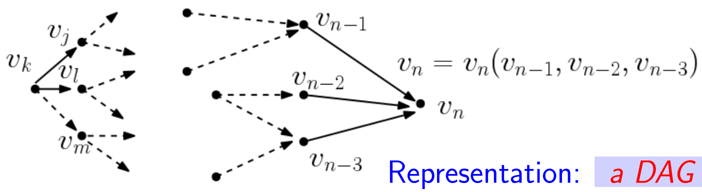
➤ Here is a very simple example from Neural Networks

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



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

Back-Propagation: General computational graphs



Representation: *a DAG*

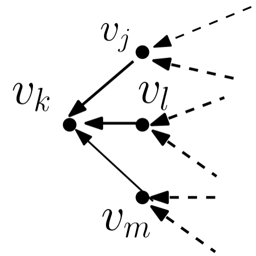
- Last node (v_n) is the target function. Let us rename it f.
- Nodes $v_i, i = 1, \cdots, e$ with indegree 0 are the variables
- Want to compute $\partial f / \partial v_1, \partial f / \partial v_2, \cdots, \partial f / \partial v_e$
- Simply use the chain rule. Look for example at node v_k in figure

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

- 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: