Graph: representation and traversal
CISC5835, Computer Algorithms
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## Outline

- Graph Definition
- Graph Representation
- Path, Cycle, Tree, Connectivity
- Graph Traversal Algorithms
- Breath first search/traversal
- Depth first search/traversal
- ...
- Minimal Spaning Tree algorithms
- Dijkstra algorithm: shortest path a


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- Slides sets by Dr. K. Wayne from Princeton
- which in turn have borrowed materials from other resources


One week of Enron emails


## Graphs - Background

Graphs = a set of nodes (vertices) with edges (links) between them.
Notations:

- $G=(V, E)$ - graph
- $V=$ set of vertices (size of $V=n$ )
- $E=$ set of edges (size of $E=m$ )

Directed graph

Undirected
graph

Acyclic graph

Some graph applications

| graph | node | edge |
| :---: | :---: | :---: |
| communication | telephone, computer | fiber optic cable |
| circuit | gate, register, processor | wire |
| mechanical | joint | rod, beam, spring |
| financial | stock, currency | transactions |
| transportation | street intersection, airport | highway, airway route |
| internet | class C network | connection |
| game | board position | legal move |
| social relationship | person, actor | friendship, movie cast |
| neural network | neuron | synapse |
| protein network | protein | protein-protein interaction |
| molecule | atom | bond |

## Other Types of Graphs

- A graph is connected if there is a path between every two vertices

- A bipartite graph is an undirected graph $G=(V, E)$ in which $V=V_{1}+V_{2}$ and there are edges only between vertices in $V_{1}$ and $V_{2}$



## Graph Representation

- Adjacency list representation of $G=(V, E)$
- An array of $n$ lists, one for each vertex in $V$
- Each list Adj[u] contains all the vertices v such that there is an edge between $u$ and $v$
- Adj[u] contains the vertices adjacent to u (in arbitrary order)
- Can be used for both directed and undirected graph


Undirected graph


Properties of Adjacency List Representation

- Sum of the lengths of all the
adjacency lists
- Directed graph: size of E (m)
- Edge ( $u, v$ ) appears only once in u's list
- Undirected graph: $2^{*}$ size of E (2m)
- $u$ and $v$ appear in each other's adjacency lists: edge ( $u, v$ ) appears twice


Undirected graph

## Graph Representation

- Memory required
- $\Theta$ (m+n)
- Preferred when
- the graph is sparse: $m \ll n^{2}$
- Disadvantage
- no quick way to determine whether there is an edge between node $u$ and $v$
- Time to determine if $(u, v)$ exists: O(degree(u))
- Time to list all vertices adjacent to u: - $\Theta$ (degree(u))


Undirected graph


- Adjacency matrix representation of $G=(V, E)$
- Assume vertices are numbered 1,2, ... n
- The representation consists of a matrix $A_{n \times n}$
$-a_{i j}= \begin{cases}1 & \text { if }(i, j) \text { belongs to } E \text {, if there is edge }(i, j)\end{cases}$ O otherwise


Undirected graph

|  | 1 | 2 | 3 | 4 | 5 | For undirected graphs matrix A is symmetric: |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 0 | 1 | 0 | 0 | 1 |  |
| 2 | 1 | 0 | 1 | 1 | 1 |  |
| 3 | 0 | 1 | 0 | 1 | 0 | $\mathrm{a}_{\mathrm{ij}}=\mathrm{a}_{\mathrm{ji}}$ |
| 4 | 0 | 1 | 1 | 0 | 1 | $\mathrm{A}=\mathrm{A}^{\top}$ |
| 5 | 1 | 1 | 0 | 1 | 0 |  |

Properties of Adjacency Matrix Representation

- Memory required
- $\Theta\left(n^{2}\right)$, independent on the number of edges in $G$
- Preferred when
- The graph is dense: $m$ is close to $n^{2}$
- need to quickly determine if there is an edge between two vertices
- Time to list all vertices adjacent to u:
$-\Theta(n)$
- Time to determine if $(u, v)$ belongs to $E:$
$-\Theta(1)$


## NetworkX: a Python graph library

- http://networkx.github.io/
- Node: any hashable object as a node. Hashable objects include strings, tuples, integers, and more.
- Arbitrary edge attributes: weights and labels can be associated with an edge.
- internal data structures: based on an adjacency lis representation and uses Python dictionary.
- adjacency structure: implemented as a dictionary of dictionaries
- top-level (outer) dictionary: keyed by nodes to values that are themselves dictionaries keyed by neighboring node to edge attributes associated with that edge.
- Support: fast addition, deletion, and lookup of nodes and neighbors in large graphs.
- underlying datastructure is accessed directly by methods


## Weighted Graphs

- Weighted graphs = graphs for which each edge has an associated weight w(u, v)
w: E-> R, weight function
- Storing the weights of a graph
- Adjacency list:
- Store $w(u, v)$ along with vertex v in u's adjacency list
- Adjacency matrix
- Store $w(u, v)$ at location ( $u, v)$ in the matrix


## Graphs Everywhere

- Prerequisite graph for CIS undergrad courses
- Three jugs of capacity 8,5 and 3 liters, initially filled with 8,0 and 0 liters respectively. How to pour water between them so that in the end we have 4,4 and 0 liters in the three jugs?
- what's this graph representing?



## Outline

## - Graph Definition

- Graph Representation
- Path, Cycle, Tree, Connectivity
- Graph Traversal Algorithms
- basis of other algorithms


## Paths

- A Path in an undirected graph $\mathrm{G}=(\mathrm{V}, \mathrm{E})$ is a sequence of nodes $v_{1}, v_{2}, \ldots, v_{k}$ with the property that each consecutive pair $v_{i-1}, v_{i}$ is joined by an edge in E .
- A path is simple if all nodes in the path are distinct.
- A cycle is a path $v_{1}, v_{2}, \ldots, v_{k}$ where $v_{1}=v_{k}, k>2$, and the first $k-1$ nodes are all distinct
- An undirected graph is connected if for every pair of nodes $u$ and $v$, there is a path between $u$ and $v$


## Rooted Trees

- Given a tree T, choose a root node r and orient each edge away from r.
- Importance: models hierarchy structure

a tree

the same tree, rooted at 1


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## Breadth-First Search (BFS)

- Input:
- A graph $G=(V, E)$ (directed or undirected)
- A source vertex s from V
- Goal:
- Explore the edges of G to "discover" every vertex reachable from $s$, taking the ones closest to $s$ first
- Output:
- $d[v]=$ distance (smallest \# of edges) from s to $v$, for all v from V
- A "breadth-first tree" rooted at s that contains all reachable vertices


## Searching in a Graph

- Graph searching = systematically follow the edges of the graph to visit all vertices of the graph
- Graph algorithms are typically elaborations of the basic graph-searching algorithms
- e.g. puzzle solving, maze walking...
- Two basic graph searching algorithms:
- Breadth-first search
- Depth-first search
- Difference: the order in which they explore unvisited edges of the graph


## Breadth-First Search (cont.)

- Keeping track of progress:
- Color each vertex in either white, gray or black
- Initially, all vertices are white
- When being discovered a vertex becomes gray
- After discovering all its adjacent
source vertices the node becomes black
- Use FIFO queue $Q$ to maintain the set of gray vertices



## Breadth-First Tree

- BFS constructs a breadth-first tree
- Initially contains root (source vertex s)
- When vertex $v$ is discovered while scanning adjacency list of $a$ vertex $u \Rightarrow$ vertex $v$ and edge $(u, v)$ are added to the source tree
- A vertex is discovered only once $\Rightarrow$ it has only one parent
- $u$ is the predecessor (parent) of $v$ in the breadth-first tre

- Breath-first tree contains nodes that are reachable from
source node, and all edges from each node's predecessor to the node


## BFS: Implementation Detail

- $G=(V, E)$ represented using adjacency lists
- color[u] - color of vertex u in V
- pred[u] - predecessor of u
- If $u=s$ (root) or node $u$ has not yet been
discovered then pred[u] = NIL
- $d[u]$ - distance (hop count) from source $s$ to source $d=1$ vertex u
- Use a FIFO queue $Q$ to maintain set of gray



## BFS Application

- BFS constructs a breadth-first tree
- BFS finds shortest (hop-count) path from src node to all other reachable nodes
- E.g., What's shortest path from 1 to 3 ?
- perform BFS using node 1 as source node
- Node 2 is discovered while exploring 1's adjacent nodes => pred. of node 2 is node 1
- Node 3 is discovered while exploring node 2's
 adjacent nodes $=>$ pred. of node 3 is node 2
- so shortest hop count path is: 1,2,3
- Useful when we want to find minimal steps to reach a state


## BFS (V, E, s)

for each $u$ in $\mathrm{V}-\{s\}$
do $\operatorname{color}[\mathrm{u}]=\mathrm{wHITE}$
$\mathrm{d}[\mathrm{u}] \leftarrow \infty$
$\operatorname{pred}[\mathrm{u}]=\mathrm{NIL}$

## BFS (V, E, s)

10. while $Q$ not empty
11. do $u \leftarrow \operatorname{DEQUEUE}(Q)$
12. for each $v$ in $\operatorname{Adj}[u]$

do if color $[\mathrm{v}]=$ WHITE
then color[ v$]=$
GRAY
$d[v] \leftarrow d[u]+1$
$\operatorname{pred}[v]=u$
ENQUEUE(Q, v)
color[u] = BLACK

## Analysis of BFS



## Example



## Analysis of BFS

10. while $Q$ not empty
11. do $u \leftarrow \operatorname{DEQUEUE}(Q) \quad \Theta(1)$
12. for each $v$ in $\operatorname{Adj}[u]$ Scan Adj[u] for all vertices
do if color $[v]=$ WHITE $\quad \begin{gathered}\text { - Each vertex } u \text { is processed } \\ \text { only once when }\end{gathered}$
then color $[\mathrm{v}]=\quad$ dequeued

- Sum of lengths of all
- Sum of lengths of all GRAY $\quad$ adjacency lists $=\Theta(|E|)$
- Scann
(|E|)

15. 

$\mathrm{d}[\mathrm{v}] \leftarrow \mathrm{d}[\mathrm{u}]+1 \quad \mathrm{O}(|\mathrm{E}|)$
$\operatorname{pred}[v]=\overleftarrow{u}(1)$
$\operatorname{ENQUEUE}(Q, v)$
18. Tofoll runiliing time for $\mathrm{BFS}=\mathrm{O}(|\mathrm{V}|+|E|)^{32}$

## Shortest Paths Property

- BFS finds the shortest-path distance from the source vertex $s \in V$ to each node in the graph
- Shortest-path distance $=d(s, u)$
- Minimum number of edges in any path from $s$ to $u$



## Depth-First Search

- Input:
- $G=(V, E)$ (No source vertex given!)
- Goal:
- Explore edges of G to "discover" every vertex in V starting at most current visited node
- Search may be repeated from multiple sources
- Output:
- 2 timestamps on each vertex:
- d[v] = discovery time (time when $v$ is first reached)
- $f[v]=$ finishing time (done with examining $v$ 's adjacency पs
- Depth-first forest


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## Depth-First Search: idea

- Search "deeper" in graph whenever possible
- explore edges of most recently discovered vertex v (that still has unexplored edges)
- After all edges of v have been explored, "backtracks" to parent of $v$
- Continue until all vertices reachable from original source have been discovered
- If undiscovered vertices remain, choose one of them as a new source and repeat search from that vertex
- different from BFS!!!
- DFS creates a "depth-first forest"



## DFS(V, E): top level

```
for each u \in V
    do color[u]}\leftarrow WHITE
            pred[u]}\leftarrow\textrm{NIL
    time }\leftarrow
for each \(u \in V\)
do if color[u] = WHITE
7. then DFS-VISIT(u)
```



- Every time DFS-VISIT(u) is called, u becomes the root of a new tree in the depth-first forest


## DFS Additional Data Structures

- Global variable: time-step
- Incremented when nodes are discovered/finished
- color[u] - color of node u

White not discovered, gray discovered and being processing and black when finished processing

- pred[u] - predecessor of u (from which node we discover u)
- d[u]- discovery (time when u turns gray)
- f[u] - finish time (time when u turns black)
$1 \leq \mathrm{d}[\mathrm{u}]<\mathrm{f}[\mathrm{u}] \leq 2|\mathrm{~V}|$



## DFS-VISIT(u): DFS exploration from u

1. color $[u] \leftarrow$ GRAY
2. time $\leftarrow$ time +1
3. $\mathrm{d}[\mathrm{u}] \leftarrow$ time
4. for each $v \in \operatorname{Adj}[u]$
5. do if color[ v$]=$ WHITE
6. then $\operatorname{pred}[v] \leftarrow u$
7. DFS-VISIT(v)
8. color $[u] \leftarrow$ BLACK //done with $u$
9. time $\leftarrow$ time +1
10. $f[u] \leftarrow$ time //finish time

time $=1$



| Example (cont.) |  |  |
| :---: | :---: | :---: |
| $\begin{aligned} & 0.0 \\ & 0.00 \end{aligned}$ | $\begin{aligned} & 0.0 \\ & 0.00 \end{aligned}$ | $\begin{aligned} & 0.0 \\ & 00 \\ & \hline 0 \end{aligned}$ |
| $\begin{aligned} & 00 \\ & 000 \\ & 000 \end{aligned}$ | oq" | $\begin{aligned} & 0.0 \\ & 0.0 \end{aligned}$ |
| $\begin{aligned} & 090 \\ & 000 \end{aligned}$ | The results of DFS may depend on:- The order in which nodes areexplored in procedure DFS- The order in which the neighbors of a |  |

## Properties of DFS

- $\quad u=\operatorname{pred}[v] \Longleftrightarrow \operatorname{DFS}-\mathrm{VISIT}(\mathrm{v})$ was called
during a search of u's adjacency list
- $\quad u$ is the predecessor (parent) of $v$
- More generally, vertex $v$ is a
descendant of vertex $u$ in depth first

forest $\Longleftrightarrow v$ is discovered while $u$ is gray


## DAG

- Directed acyclic graphs (DAGs)
- Used to represent precedence of events or processes that have a partial order


Topological sort helps us establish a total order/ linear order. Useful for task scheduling.


## Topological Sort



TOPOLOGICAL-SORT(V, E)

1. Call DFS(V, E) (to compute finishing times $f[v]$ for each vertex $v$ ): when a node is finished, push it on to a stack
2. pop nodes in stack and arrange them in a list

Running time: $\Theta(|\mathrm{V}|+|E|)$
watch shirt belt tie jacket socks undershorts pants shoes

## Topological Sort via DFS



Consider when DFS visit(undershorts) is called, jacket is either

* white: then jacket will be discovered in DFS_visit(undershorts), turn black, before eventually undershorts finishes. ffjacket] < flundershorts]
* black (if DFS_visit(jacket) was called): then fljacket] < flundershorts]
* node jacket cannot be gray (which would mean that DFS_visit(jacket) is ongoing ...)


## Edge Classification*

- Via DFS traversal, graph edges can be classified into four types.
- When in DFS_visit (u), we follow edge ( $u, v$ ) and find node, if $v$ is:
- WHITE vertex: then ( $u, v$ ) is a tree edge
a depth first tree
- Self loops (in directed graphs) are also back edges

$(x, v)$ is a back edge
- $v$ was first discovered by exploring edge (u, v)
- GRAY node: then $(u, v)$ is a Back edge
- ( $u, v$ ) connects $u$ to an ancestor $v$ in


## Edge Classification*

- if $v$ is black vertex, and $d[u]<\mathrm{d}[\mathrm{v}],(\mathrm{u}, \mathrm{v})$ is a Forward edge ( $u, v$ ):
- Non-tree edge (u, v) that connects a vertex $u$ to a descendant $v$ in a depth first tree

$(u, x)$ is a forward edge


## Cross edge ( $u, v$ ):

- go between vertices in same depth-first tree (as long as there is no ancestor /
descendant relation) or between different depth-first trees



## Analysis of DFS-VISIT(u)

1. color $[u] \leftarrow$ GRAY

DFS-VISIT is called exactly once for each vertex
2. time $\leftarrow$ time +1
3. $d[u] \leftarrow$ time
4. for each $v \in \operatorname{Adj}[u]$
5. do if color[v] = WHITE
6. $\quad$ then $\operatorname{pred}[v] \leftarrow u$

Each loop takes |Adj[u]|

DFS-VISIT(v)
)

## Analysis of DFS (V, E)

1. for each $u \in V$
$\left.\begin{array}{ll}\text { 2. do color }[u] \leftarrow \text { WHITE } \\ \text { 3. } & \operatorname{pred}[u] \leftarrow \mathrm{NIL}\end{array}\right\} \quad \Theta(|\mathrm{V}|)$
2. time $\leftarrow 0$
3. for each $u \in V \quad \Theta(|V|)-$ without
4. do if color $[u]=$ WHITE
5. then DFS-VISIT(u) for DFS-VISIT

## DFS without recursion*

Data Structure: use stack (Last In First Out!)
to store all gray nodes

## Pseudocode:

1. Start by push source node to stack
2. Explore node at stack top, i.e

* push its next white adj. node to stack)
* if all its adj nodes are black, the node turns black, pop it from stack 3. Continue (go back 2) until stack is empty

4. If there are white nodes remaining, go back to 1 using another white node as source node
5. color $[u] \leftarrow$ BLACK
6. time $\leftarrow$ time +1 Total: $\Sigma_{u \in V}|\operatorname{Adj}[u]|+\Theta(|V|)=$

$$
\text { 10. } \mathrm{f}[\mathrm{u}] \leftarrow \text { time } \quad \underbrace{}_{\Theta(|\mathrm{E}|)}=\Theta(|\mathrm{V}|+|E|)
$$



## Cycle detection via DFS

A directed graph is acyclic $\Longleftrightarrow$ a DFS on $G$ yields no back edges.

## Proof:

" $\Rightarrow$ ": acyclic $\Rightarrow$ no back edge

- Assume back edge $\Rightarrow$ prove cycle
- Assume there is a back edge ( $u, v$ )
$\Rightarrow v$ is an ancestor of $u$
$\Rightarrow$ there is a path from $v$ to $u$ in $G(v \Rightarrow u)$
$(u, v) \int_{0}^{v}$
$\Rightarrow v \Rightarrow \quad u+$ the back edge $(u, v)$ yield a cycle


## Other Properties of DFS*

## Corollary

Vertex $v$ is a proper descendant of $u$
$\Longleftrightarrow d[u]<d[v]<f[v]<f[u]$


Theorem (White-path Theorem)
In a depth-first forest of a graph G, vertex $v$ is a descendant of $u$ if and only if at time $d[u]$, there is a path $u \Rightarrow v$
consisting of only white vertices.


## Shortest Distance Paths

- Distance/Cost of a path in weighted graph
- sum of weights of all edges on the path
- path $\mathrm{A}, \mathrm{B}, \mathrm{E}$, cost is $2+3=5$
- path $A, B, C, E$, cost is $2+1+4=7$

- How to find shortest distance path from a node, A , to all another node?
- assuming: all weights are positive
- This implies no cycle in the shortest distance path
- Why? Prove by contradiction.
- If $A->B->C->$...>B->D is shortest path, then $A->B->D$ is a shorter!
- d[u]: the distance of the shortest-distance path from $A$ to $u$
$\mathrm{d}[\mathrm{A}]=0$
$d[D]=\min \{d[B]+2, d[E]+2\}$
because $B, E$ are the two only possible previous node in path to $D$


## Dijkstra Algorithm

Input: positive weighted graph G, source node s

- Output: shortest distance path from s to all other nodes that is reachable from s

Expanding frontier (one hop a time)
1). Starting from $A$ :

We can go to $B$ with cost $B$, go to $C$ with cost 1

going to all other nodes (here $D, E$ ) has to pass $B$ or $C$ are there cheaper paths to go to C ?
are there cheaper paths to B ?
2). Where can we go from $C$ ? $B, E$

Two new paths: (A,C,B) ( $A, C, E$ )
Better paths than before? => update current optimal path there cheaper paths to $B$ ?
3). Where can we go from $B$ ?
for each node $u$, keep track pred[u] (previous node in the path leading to $u$ ), $\mathrm{d}[u]$ current shortest distance


## Dijkstra's algorithm \& snapshot

procedure dijkstra( $G, l, s$ )
Input: Graph $G=(V, E)$, directed or undirected;
Output: For all vertices $u$ reachable from $s$, $\operatorname{dist}(u)$ is set to the distance from $s$ to $u$.
for all $u \in V$ :
$\operatorname{dist}(u)=\infty$
$\operatorname{prev}(u)=$ nil
$\operatorname{dist}(s)=0$

## H : priority queue (min-heap in this case)

$H=$ makequeue $(V) \quad$ (using dist-values as keys) prev=A prev=nil while $H$ is not empty
for all edges $(u, v) \in E$ :
if $\operatorname{dist}(v)>\operatorname{dist}(u)+l(u, v)$ : $\operatorname{dist}(v)=\operatorname{dist}(u)+l(u, v)$ $\operatorname{prev}(v)=u$
decreasekey $(H, v)$


## Formal Definition of MST

- Given a connected, undirected, weighted graph $G=(V, E)$, a spanning tree is an acyclic subset of edges $T \subseteq E$ that connects all vertices together.
- cost of a spanning tree $T$ : the sum of edge weights in the spanning tree

$$
w(T)=\sum_{(u, v) \in T} w(u, v)
$$

- A minimum spanning tree (MST) is a spanning tree of minimum weight.


## Minimum Spanning Trees

- Minimum Spanning Tree Problem: Given a weighted graph, choose a subset of edges so that resulting subgraph is connected, and the total weights of edges is minimized
- to minimize total weights, it never pays to have cycles, so resulting connection graph is connected, undirected, and acyclic, i.e., a tree.
- Applications:
- Communication networks
- Circuit design
- Layout of highway systems



## Minimum Spanning Trees

- Given: Connected, undirected, weighted graph, G
- Find: Minimum - weight spanning tree, $T$


Acyclic subset of edges(E) that connects all vertices of $G$

Notice: there are many spanning trees for a graph We want to find the one with the minimum cost

Such problems are optimization problems: there are multiple viable solutions, we want to find best (lowest cost, best perf) one.

## Greedy Algorithms

- A problem solving strategy (like divide-and-conquer)
- Idea: build up a solution piece by piece, in each step always choose the option that offers best immediate benefits (a myopic approach)
- Local optimization: choose what seems best right now
- not worrying about long term benefits/global benefits
- Sometimes yield optimal solution, sometimes yield suboptimal (i.e., not optimal)
- Sometimes we can bound difference from optimal...


## Kruskal's Algorithm

## Figure 5.4 Kruskal's minimum spanning tree algorithm.

procedure kruskal ( $G, w$ )
Input: A connected undirected graph $G=(V, E)$ with edge weights $w_{e}$
utput: A minimum spanning tree defined by the edges
for all $u \in V$
$\operatorname{makeset}(u)$
$X=\{ \}$
ort the edges $E$ by weight
for all edges $\{u, v\} \in E$, in increasing order of weight
f find $(u) \neq \mathrm{f}$ ind $(v)$ :
union $(u, v)$
Implementation detail:

* Maintain sets of nodes that are connected by tree edges
* find(u): return the set that $u$ belongs to
* find(u)=find(v) means $u$, v belongs to same group (i.e., $u$ and $v$ are already connected)


## Minimum Spanning Trees

- Given: Connected, undirected, weighted graph, G
- Find: Minimum - weight spanning tree, $T$


How to greedily build a spanning tree?
*Always choose lightest edge? Might lead to cycle.

* Repeat for n-1 times:
find next lightest edge that does not introduce cycle.
add the edge into tree
=> Kruskal's algorithm


## Minimum Spanning Trees

- Given: Connected, undirected, weighted graph, G
- Find: Minimum - weight spanning tree, $T$



## Example:

Suppose we start grow tree from C
step 1. A has lightest edge to tree, add A
and the edge $(A-C)$ to tree
// tree is now A-C
step 2: D has lightest edge to tree add $D$ and the edge ( $C-D$ ) to tree

How to greedily build a spanning tree?

* Grow the tree from a node (any node),
* Repeat for n-1 times:
* connect one node to the tree by choosing node with lightest edge connecting to tree nodes

This is Prim algorithm.

## Prim's Algorithm

Input: A connected undirected graph $G=(V, E)$ with edge weights $w_{e}$ Output: A minimum spanning tree defined by the array prev


## Summary

- Graph everywhere: represent binary relation
- Graph Representation
- Adjacent lists, Adjacent matrix
- Path, Cycle, Tree, Connectivity
- Graph Traversal Algorithm: systematic way to explore graph (nodes)
- BFS yields a fat and short tree
- App: find shortest hop path from a node to other nodes
- DFS yields forest made up of lean and tall tree
- App: detect cycles and topological sorting (for DAG)

