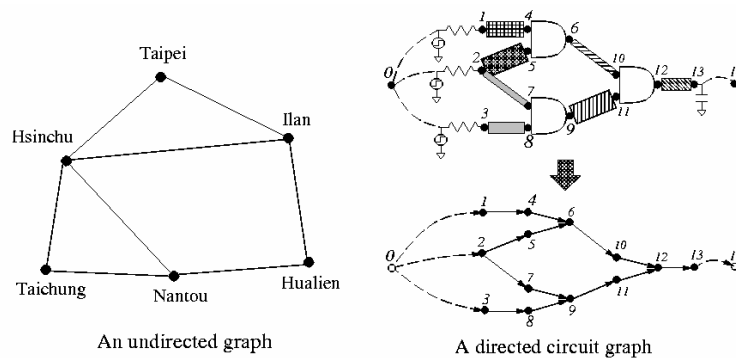


Unit 2: Algorithmic Graph Theory

- Course contents:
 - Introduction to graph theory
 - Basic graph algorithms
- Reading
 - Chapter 3
 - Reference: Cormen, Leiserson, and Rivest, *Introduction to Algorithms*, 2nd Ed., McGraw Hill/MIT Press, 2001.



Unit 2

NTUEE/ Intro. EDA

1

Algorithms

- **Algorithm:** A well-defined procedure for transforming some **input** to a desired **output**.
- **Major concerns:**
 - **Correctness:** Does it **halt**? Is it **correct**?
 - **Efficiency:** **Time** complexity? **Space** complexity?
 - Worst case? Average case? (Best case?)
- **Better algorithms?**
 - **How:** **Faster** algorithms? Algorithms with **less space** requirement?
 - **Optimality:** Prove that an algorithm is **best possible/optimal**? Establish a **lower bound**?

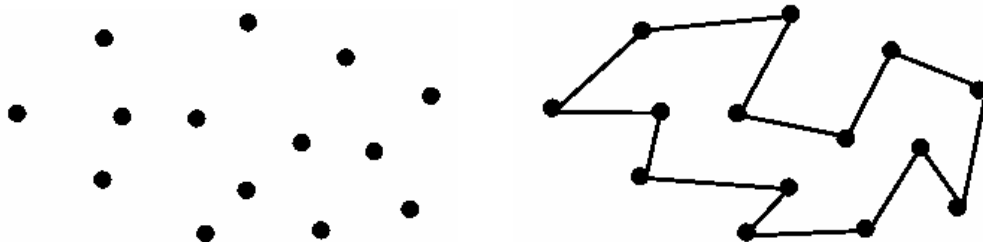
Unit 2

NTUEE/ Intro. EDA

2

Example: Traveling Salesman Problem (TSP)

- **Instance:** A set of points (cities) P together with a distance $d(p, q)$ between any pair $p, q \in P$.
- **Output:** What is the shortest circular route that starts and ends at a given point and visits all the points.

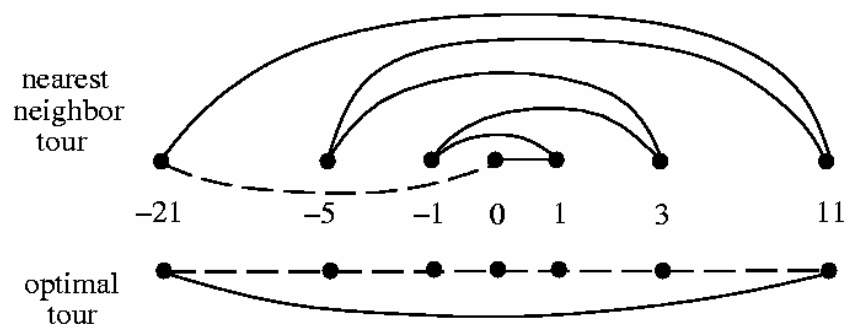


- Correct and efficient algorithms?

Nearest Neighbor Tour

1. pick and visit an initial point p_0 ;
2. $P \leftarrow p_0$;
3. $i \leftarrow 0$;
4. **while** there are unvisited points **do**
5. visit p_i 's closet unvisited point p_{i+1} ;
6. $i \leftarrow i + 1$;
7. return to p_0 from p_i .

- Simple to implement and very efficient, but **incorrect!**



A Correct, but Inefficient Algorithm

```
1.  $d \leftarrow \infty$  ;
2. for each of the  $n!$  permutations  $\pi_j$  of the  $n$  points
3.   if  $(\text{cost}(\pi_j) \leq d)$  then
4.      $d \leftarrow \text{cost}(\pi_j)$ ;
5.      $T_{min} \leftarrow \pi_j$ ;
6. return  $T_{min}$ .
```

- **Correctness:** Tries all possible orderings of the points \Rightarrow Guarantees to end up with the shortest possible tour.
- **Efficiency:** Tries $n!$ possible routes!
 - 120 routes for 5 points, 3,628,800 routes for 10 points, 20 points?
- No known efficient, correct algorithm for TSP!

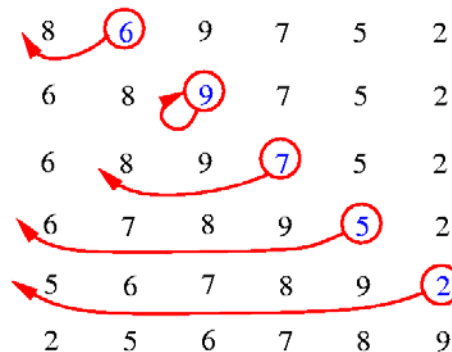
Example: Sorting

- **Instance:** A sequence of n numbers $\langle a_1, a_2, \dots, a_n \rangle$.
- **Output:** A permutation $\langle a_1', a_2', \dots, a_n' \rangle$ such that $a_1' \leq a_2' \leq \dots \leq a_n'$.
 - Input: $\langle 8, 6, 9, 7, 5, 2, 3 \rangle$
 - Output: $\langle 2, 3, 5, 6, 7, 8, 9 \rangle$
- Correct and efficient algorithms?

Insertion Sort

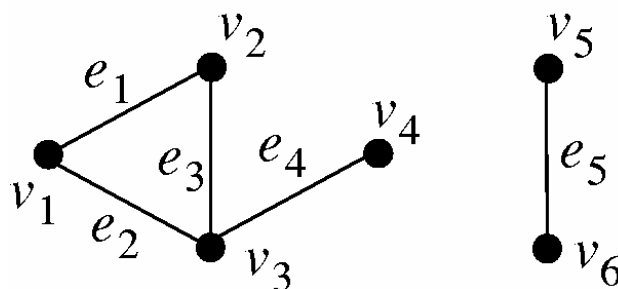
InsertionSort(A)

```
1. for  $j \leftarrow 2$  to  $\text{length}[A]$  do
2.    $\text{key} \leftarrow A[j]$ ;
3.   /* Insert  $A[j]$  into the sorted sequence  $A[1..j-1]$ . */
4.    $i \leftarrow j - 1$ ;
5.   while  $i > 0$  and  $A[i] > \text{key}$  do
6.      $A[i+1] \leftarrow A[i]$ ;
7.      $i \leftarrow i - 1$ ;
8.    $A[i+1] \leftarrow \text{key}$ ;
```



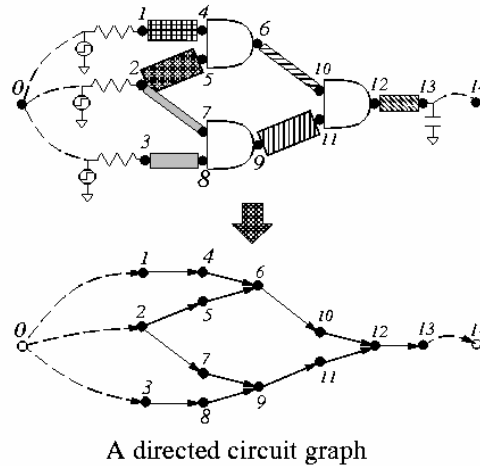
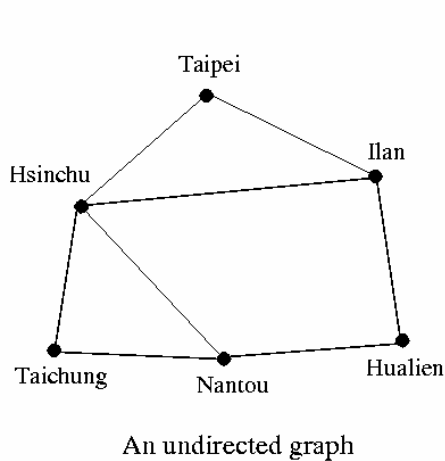
Graph

- **Graph:** A mathematical object representing a set of “points” and “interconnections” between them.
- A **graph** $G = (V, E)$ consists of a set V of **vertices** (**nodes**) and a set E of **directed** or **undirected edges**.
 - V is the vertex set: $V = \{v_1, v_2, v_3, v_4, v_5, v_6\}$, $|V|=6$
 - E is the edge set: $E = \{e_1, e_2, e_3, e_4, e_5\}$, $|E|=5$
 - An edge has two endpoints, e.g. $e_1 = (v_1, v_2)$
 - For simplicity, use V for $|V|$ and E for $|E|$.

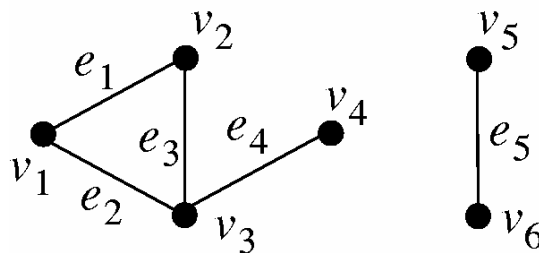


Example Graphs

- Any binary relation is a graph.
 - Network of roads and cities
 - Circuit representation



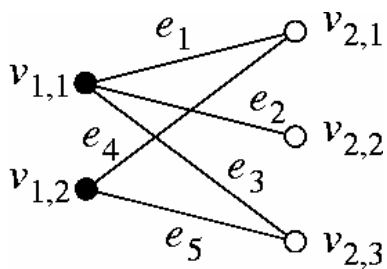
Terminology



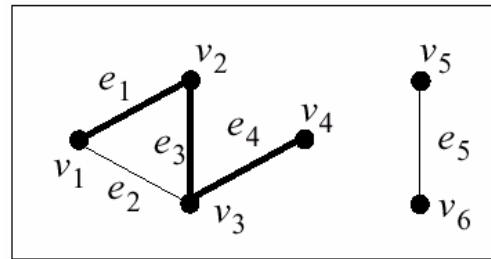
- **Degree of a vertex:** $\text{degree}(v_3) = 3$, $\text{degree}(v_2) = 2$
- **Subgraph of a graph:**
- **Complete (sub)graph:** $V = \{v_1, v_2, v_3\}$, $E = \{e_1, e_2, e_3\}$
- **(Maximal/maximum) clique:** maximal/maximum complete subgraph
- **Selfloop**
- **Parallel edges**
- **Simple graph**
- **Multigraph**

Terminology (cont'd)

- Bipartite graph $G = (V_1, V_2, E)$
- Path
- Cycle: a closed path
- Connected vertices
- Connected graph
- Connected components



A bipartite graph

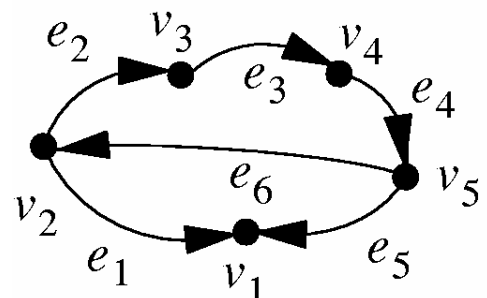


Path $p = \langle v_1, v_2, v_3, v_4 \rangle$

Cycle $C = \langle v_1, v_2, v_3, v_1 \rangle$

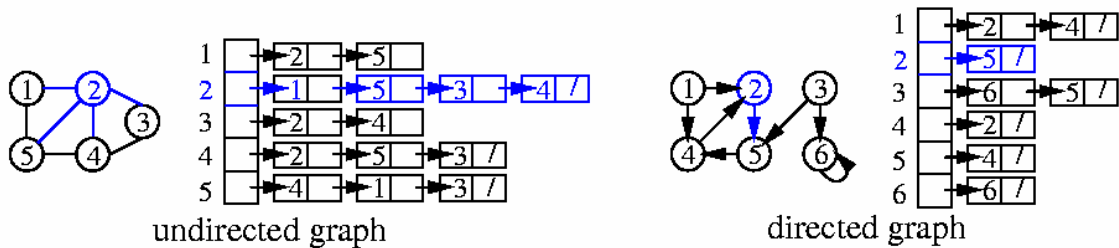
Terminology (cont'd)

- **Weighted graph:**
 - Edge weighted and/or vertex weighted
- **Directed graph:** edges have directions
 - Directed path
 - Directed cycle
 - Directed acyclic graph (DAG)
 - In-degree, out-degree
 - Strongly connected vertices
 - Strongly connected components $\{v_1\}\{v_2, v_3, v_4, v_5\}$
 - Weakly connected vertices



Graph Representation: Adjacency List

- **Adjacency list:** An array Adj of $|V|$ lists, one for each vertex in V . For each $u \in V$, $Adj[u]$ pointers to all the vertices adjacent to u .
- Advantage: $O(V+E)$ storage, good for **sparse** graph.
- Drawback: Need to traverse list to find an edge.

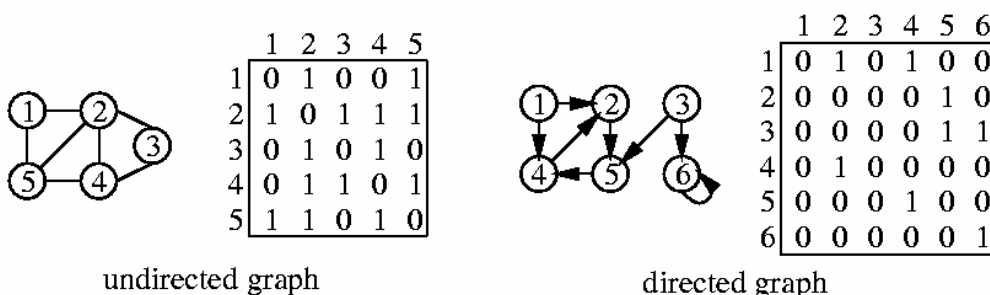


Graph Representations: Adjacency Matrix

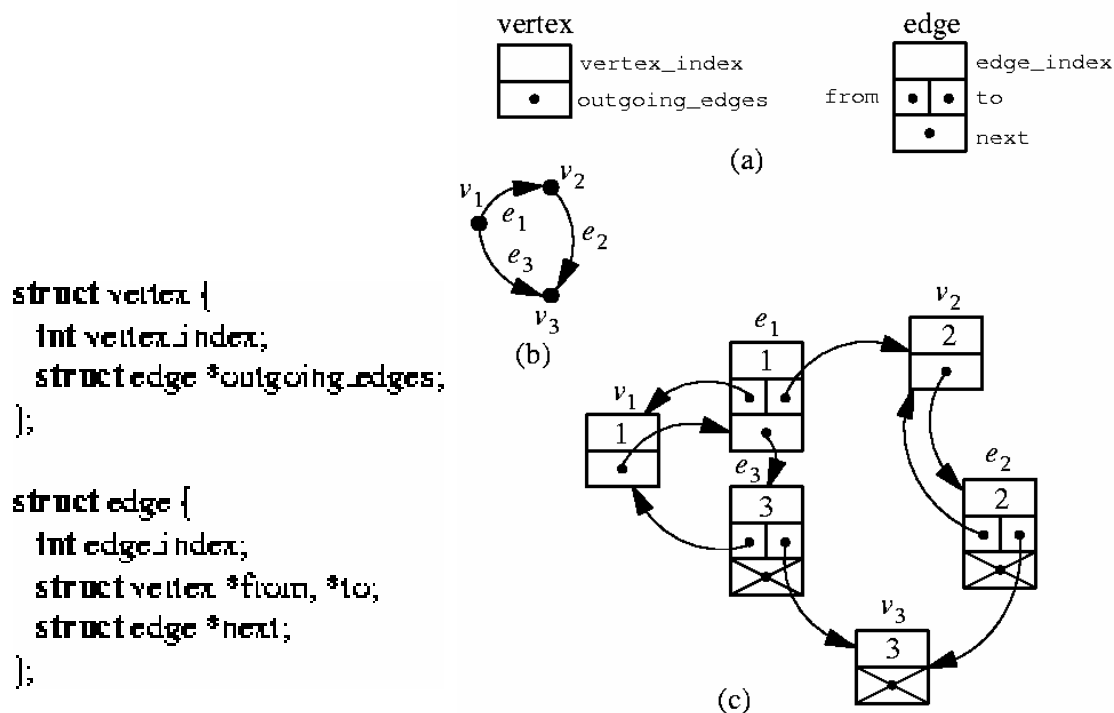
- **Adjacency matrix:** A $|V| \times |V|$ matrix $A = (a_{ij})$ such that

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

- Advantage: $O(1)$ time to find an edge.
- Drawback: $O(V^2)$ storage, suitable for **dense** graph.
- How to save space if the graph is undirected?



Explicit Edges and Vertices



Tradeoffs between Adjacency List and Matrix

Comparison	Winner
Faster to find an edge?	matrix
Faster to find vertex degree?	list
Faster to traverse the graph?	list $O(V + E)$ vs. matrix $O(V^2)$
Storage for sparse graph?	list $O(V + E)$ vs. matrix $O(V^2)$
Storage for dense graph?	matrix (small win)
Edge insertion or deletion?	matrix $O(1)$
Weighted-graph implementation?	?
Better for most applications?	list

Depth-First Search (DFS) [Cormen]

DFS(G)

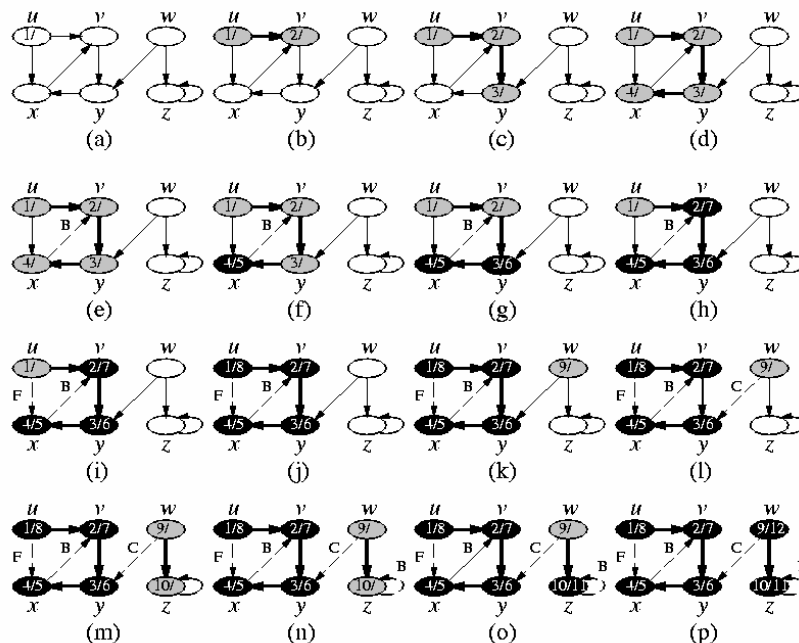
1. **for** each vertex $u \in V[G]$
2. $color[u] \leftarrow WHITE$;
3. $\pi[u] \leftarrow NIL$;
4. $time \leftarrow 0$;
5. **for** each vertex $u \in V[G]$
6. **if** $color[u] = WHITE$
7. DFS-Visit(u).

DFS-Visit(u)

1. $color[u] \leftarrow GRAY$;
- /* White vertex u has just been discovered. */
2. $d[u] \leftarrow time \leftarrow time + 1$;
3. **for** each vertex $v \in Adj[u]$
- /* Explore edge (u, v) . */
4. **if** $color[v] = WHITE$
5. $\pi[v] \leftarrow u$;
6. DFS-Visit(v);
7. $color[u] \leftarrow BLACK$;
- /* Blacken u ; it is finished. */
8. $f[u] \leftarrow time \leftarrow time + 1$.

- $color[u]$:
 - white (undiscovered) \rightarrow
 - gray (discovered) \rightarrow
 - black (explored: out edges are all discovered)
- $d[u]$: discovery time (gray)
- $f[u]$: finishing time (black)
- $\pi[u]$: predecessor
- Time complexity: $O(V+E)$ (adjacency list).

DFS Example [Cormen]



- $color[u]$: white \rightarrow gray \rightarrow black.
- Depth-first forest: $G_\pi = (V, E_\pi)$, $E_\pi = \{(\pi[v], v) \in E \mid v \in V, \pi[v] \neq NIL\}$
 – $\{u \rightarrow v \rightarrow x \rightarrow y\} \{w \rightarrow z\}$

DFS Pseudo Code in Text

```

/* Given is the graph  $G(V, E)$  */

struct vertex {
    ...
    int mark;
};

dfs(struct vertex v)
{
    v.mark ← 0;
    "process v";
    for each  $(v, u) \in E$  {
        "process  $(v, u)$ ";
        if (u.mark)
            dfs(u);
    }
}

main ()
{
    for each  $v \in V$ 
        v.mark ← 1;
    for each  $v \in V$ 
        if (v.mark)
            dfs(v);
}

```

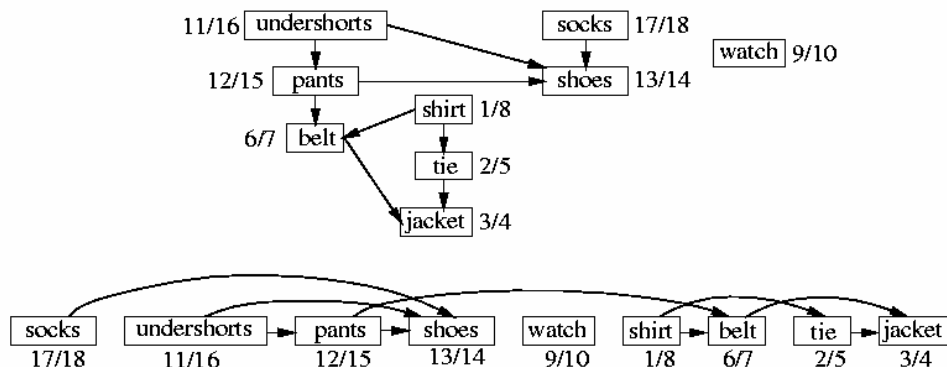
DFS Application 1: Topological Sort

- A **topological sort** of a directed acyclic graph (DAG) $G = (V, E)$ is a linear ordering of V s.t. $(u, v) \in E \Rightarrow u$ appears before v .

Topological-Sort(G)

1. call DFS(G) to compute finishing times $f[v]$ for each vertex v
2. as each vertex is finished, insert it onto the front of a linked list
3. **return** the linked list of vertices

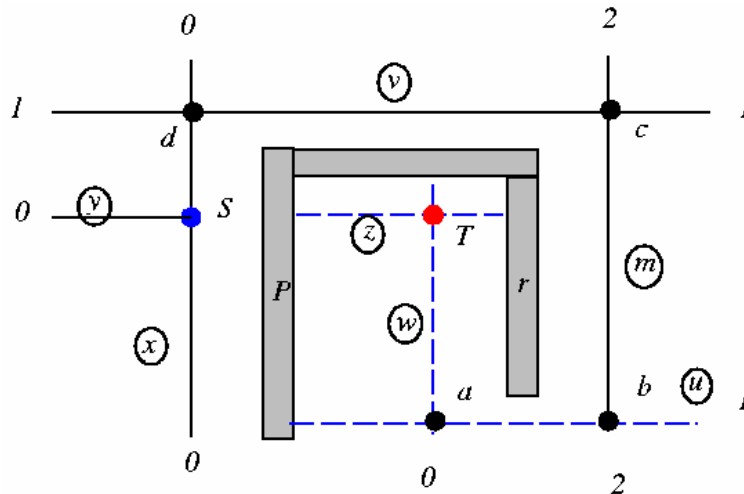
- Time complexity: $O(V+E)$ (adjacent list).



Vertices are arranged from left to right in order of decreasing finishing times.

DFS Application 2: Hightower's Maze Router

- A single escape point on each line segment.
- If a line parallels to the blocked cells, the escape point is placed just past the endpoint of the segment.
- Time and space complexities: $O(L)$, where L is the # of line segments generated.



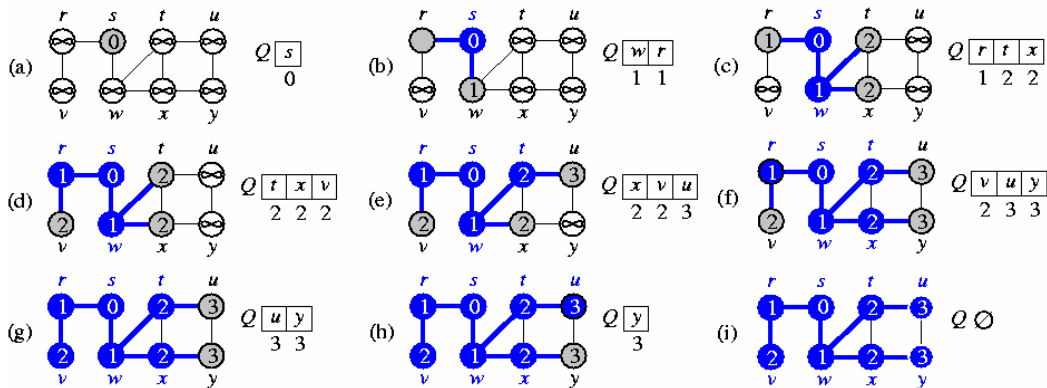
Breadth-First Search (BFS) [Cormen]

BFS(G, s)

1. **for** each vertex $u \in V[G] - \{s\}$
2. $color[u] \leftarrow WHITE$;
3. $d[u] \leftarrow \infty$;
4. $\pi[u] \leftarrow NIL$;
5. $color[s] \leftarrow GRAY$;
6. $d[s] \leftarrow 0$;
7. $\pi[s] \leftarrow NIL$;
8. $Q \leftarrow \{s\}$;
9. **while** $Q \neq \emptyset$
10. $u \leftarrow head[Q]$;
11. **for** each vertex $v \in Adj[u]$
12. **if** $color[v] = WHITE$
13. $color[v] \leftarrow GRAY$;
14. $d[v] \leftarrow d[u] + 1$;
15. $\pi[v] \leftarrow u$;
16. Enqueue(Q, v);
17. Dequeue(Q);
18. $color[u] \leftarrow BLACK$.

- $color[u]$:
 - white (undiscovered) \rightarrow
 - gray (discovered) \rightarrow
 - black (explored: out edges are all discovered)
- $d[u]$: distance from source s
- $\pi[u]$: predecessor of u
- Use queue for gray vertices
- Time complexity: $O(V+E)$ (adjacency list).

BFS Example [Cormen]



- Use queue for gray vertices.
 - Each vertex is enqueued and dequeued once: $O(V)$ time.
 - Each edge is considered once: $O(E)$ time.
- Breadth-first tree:
 - $G_\pi = (V_\pi, E_\pi)$, $V_\pi = \{v \in V \mid \pi[v] \neq \text{NIL}\} \cup \{s\}$
 - $\{s, w, r, t, x, v, u, y\}$
 - $E_\pi = \{(\pi[v], v) \in E \mid v \in V_\pi - \{s\}\}$.
 - $\{(s,w), (s,r), (w,t), (w,x), (r,v), (t,u), (x,y)\}$

BFS Pseudo Code in Text

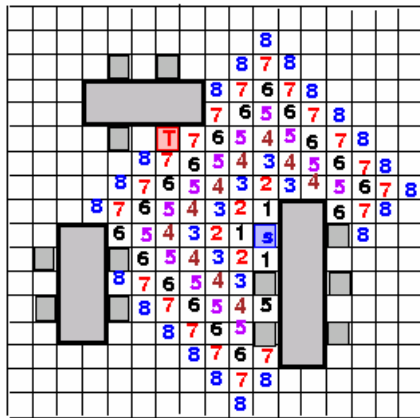
```

main ()
{
    for each  $v \in V$ 
         $v.\text{mark} \leftarrow 1$ ;
    for each  $v \in V$ 
        if ( $v.\text{mark}$ ) {
             $v.\text{mark} \leftarrow 0$ ;
            bfs( $v$ );
        }
}

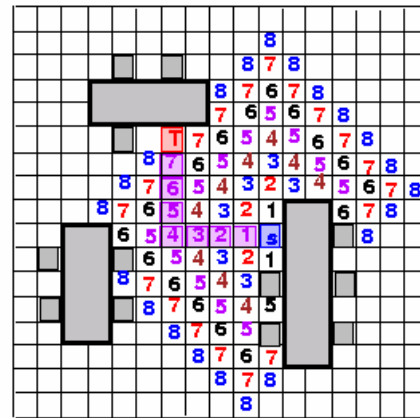
bfs(struct vertex  $v$ )
{
    struct fifo * $Q$ ;
    struct vertex  $u, w$ ;
     $Q \leftarrow ()$ ;
    shift_in( $Q, v$ );
    do {  $w \leftarrow \text{shift\_out}(Q)$ ;
        "process  $w$ ";
        for each  $(w, u) \in E$  {
            "process  $(w, u)$ ";
            if ( $u.\text{mark}$ ) {
                 $u.\text{mark} \leftarrow 0$ ;
                shift_in( $Q, u$ );
            }
        }
    } while ( $Q \neq ()$ )
}
    
```

BFS Application: Lee's Maze Router

- Find a path from S to T by “wave propagation.”
- Discuss mainly on single-layer routing
- Strength: Guarantee to find a minimum-length connection between 2 terminals if it exists.
- Weakness: Time & space complexity for an $M \times N$ grid: $O(MN)$ (huge!)



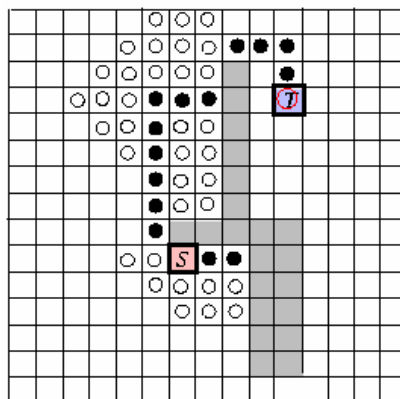
Filing



Retrace

BFS + DFS Application: Soukup's Maze Router

- **Depth-first (line) search** is first directed toward target T until an obstacle or T is reached.
- **Breadth-first (Lee-type) search** is used to “bubble” around an obstacle if an obstacle is reached.
- Time and space complexities: $O(MN)$, but 10--50 times faster than Lee's algorithm.
- Find *a* path between S and T , but may not be the shortest!



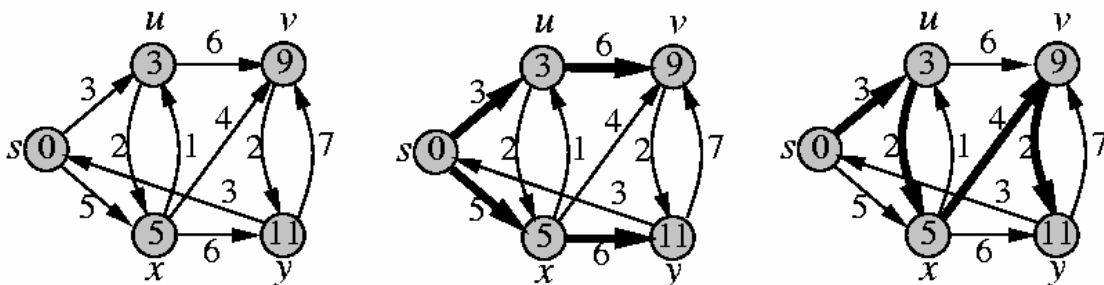
Shortest Paths (SP)

- **The Shortest Path (SP) Problem**

- **Given:** A **directed** graph $G=(V, E)$ with edge weights, and a specific **source node** s .
- **Goal:** Find a minimum weight path (or cost) from s to every other node in V .

- Applications: weights can be distances, times, wiring cost, delay. etc.

- **Special case:** BFS finds shortest paths for the case when all edge weights are 1.



Weighted Directed Graph

- A weighted, directed graph $G = (V, E)$ with the weight function $w: E \rightarrow \mathbb{R}$.

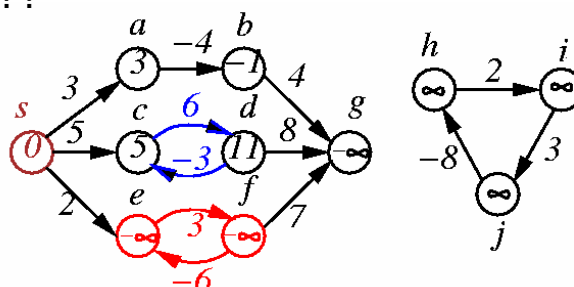
- Weight of path $p = \langle v_0, v_1, \dots, v_k \rangle$: $w(p) = \sum_{i=1}^k w(v_{i-1}, v_i)$.
- **Shortest-path weight** from u to v , $\delta(u, v)$:

$$\delta(u, v) = \begin{cases} \min\{w(p) : u \xrightarrow{p} v\} & \text{if there is a path from } u \text{ to } v, \\ \infty & \text{otherwise.} \end{cases}$$

- **Warning!** negative-weight edges/cycles are a problem.

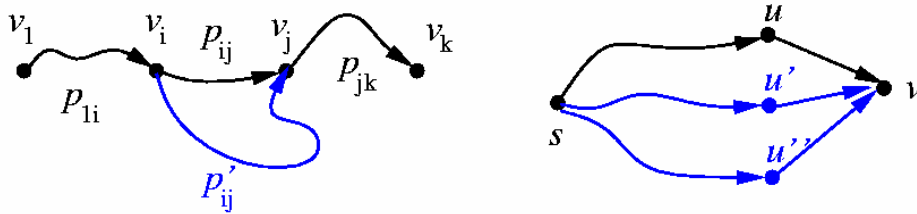
- Cycle $\langle e, f, e \rangle$ has weight $-3 < 0 \Rightarrow \delta(s, g) = -\infty$.
- Vertices h, i, j not reachable from $s \Rightarrow \delta(s, h) = \delta(s, i) = \delta(s, j) = \infty$.

- Algorithms apply to the cases for negative-weight edges/cycles??



Optimal Substructure of a Shortest Path

- Subpaths of shortest paths are shortest paths.
 - Let $p = \langle v_1, v_2, \dots, v_k \rangle$ be a shortest path from vertex v_1 to vertex v_k , and $p_{ij} = \langle v_i, v_{i+1}, \dots, v_j \rangle$ be the subpath of p from vertex v_i to vertex v_j , $1 \leq i \leq j \leq k$. Then, p_{ij} is a shortest path from v_i to v_j . (NOTE: reverse is not necessarily true!)
- Suppose that a shortest path p from a source s to a vertex v can be decomposed into $s \xrightarrow{p'} u \rightarrow v$. Then, $\delta(s, v) = \delta(s, u) + w(u, v)$.
- For all edges $(u, v) \in E$, $\delta(s, v) \leq \delta(s, u) + w(u, v)$.



subpaths of shortest paths

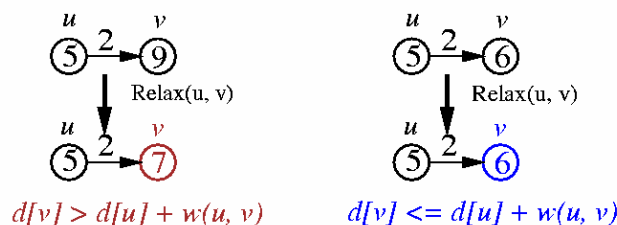
Relaxation

```

Initialize-Single-Source(G, s)
1. for each vertex v ∈ V[G]
2.  d[v] ← ∞;
   /* upper bound on the weight of a shortest path from s to v */
3.  π[v] ← NIL; /* predecessor of v */
4.  d[s] ← 0;

Relax(u, v, w)
1. if d[v] > d[u] + w(u, v)
2.  d[v] ← d[u] + w(u, v);
3.  π[v] ← u;
    
```

- $d[v] \leq d[u] + w(u, v)$ after calling $\text{Relax}(u, v, w)$.
- $d[v] \geq \delta(s, v)$ during the relaxation steps; **once $d[v]$ achieves its lower bound $\delta(s, v)$, it never changes.**
- Let $s \rightsquigarrow u \rightarrow v$ be a shortest path. If $d[u] = \delta(s, u)$ prior to the call $\text{Relax}(u, v, w)$, then $d[v] = \delta(s, v)$ after the call.



Dijkstra's Shortest-Path Algorithm

Dijkstra(G, w, s)

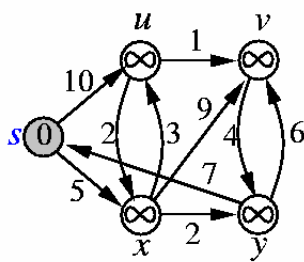
1. Initialize-Single-Source(G, s);
2. $S \leftarrow \emptyset$;
3. $Q \leftarrow V[G]$;
4. **while** $Q \neq \emptyset$
5. $u \leftarrow \text{Extract-Minimum-Element}(Q)$;
6. $S \leftarrow S \cup \{u\}$;
7. **for** each vertex $v \in \text{Adj}[u]$
8. Relax(u, v, w);

- Idea:

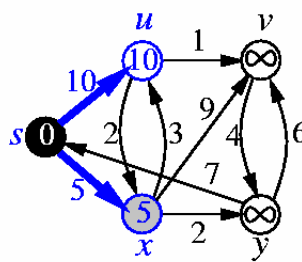
- search all shortest paths
 - In a smart way (use dynamic-programming, see next lecture)
- Then choose a shortest path

Example: Dijkstra's Shortest-Path Algorithm

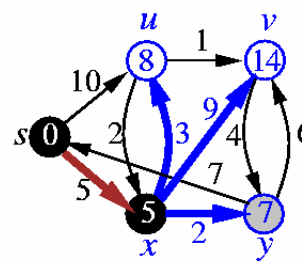
- Find the shortest path from vertex s to vertex v
 - $s \rightarrow x \rightarrow u \rightarrow v$; Weight = $5+3+1$



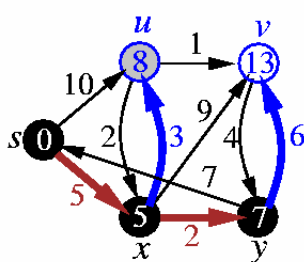
(a)



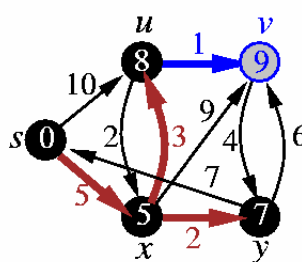
(b)



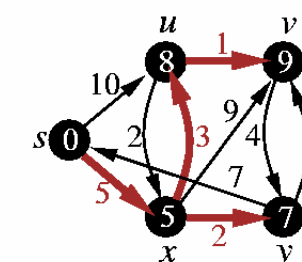
(c)



(d)



(e)



(f)

Runtime Analysis of Dijkstra's Algorithm

```
Dijkstra( $G, w, s$ )
1. Initialize-Single-Source( $G, s$ );
2.  $S \leftarrow \emptyset$ ;
3.  $Q \leftarrow V[G]$ ;
4. while  $Q \neq \emptyset$ 
5.    $u \leftarrow \text{Extract-Minimum-Element}(Q)$ ;
6.    $S \leftarrow S \cup \{u\}$ ;
7.   for each vertex  $v \in \text{Adj}[u]$ 
8.     Relax( $u, v, w$ );
```

- Q is implemented as a linear array: $O(V^2)$.
 - Line 5: $O(V)$ for Extract-Minimum-Element, so $O(V^2)$ with the **while** loop.
 - Lines 7--8: $O(E)$ operations, each takes $O(1)$ time.
- Q is implemented as a binary heap: $O(E \lg V)$.
- Q is implemented as a Fibonacci heap: $O(E + V \lg V)$.

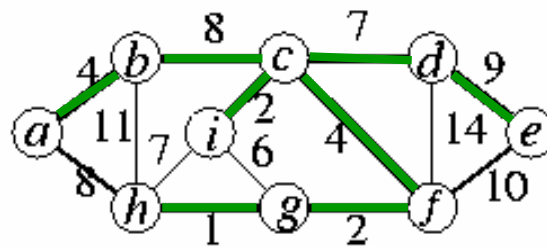
Dijkstra's SP Pseudo Code in Text

```
struct vertex {
  ...
  int distance;
};

dijkstra(set of struct vertex  $V$ , struct vertex  $v_s$ , struct vertex  $v_t$ )
{
  set of struct vertex  $T$ ;
  struct vertex  $u, v$ ;
   $V \leftarrow V \setminus \{v_s\}$ ;
   $T \leftarrow \{v_s\}$ ;
   $v_s.\text{distance} \leftarrow 0$ ;
  for each  $u \in V$ 
    if  $((v_s, u) \in E)$ 
       $u.\text{distance} \leftarrow w((v_s, u))$ 
    else  $u.\text{distance} \leftarrow +\infty$ ;
  while  $(v_t \notin T)$  {
     $u \leftarrow$  “ $u \in V$ , such that  $\forall v \in V : u.\text{distance} \leq v.\text{distance}$ ”;
     $T \leftarrow T \cup \{u\}$ ;
     $V \leftarrow V \setminus \{u\}$ ;
    for each  $v$  “such that  $(u, v) \in E$ ”
      if  $(v.\text{distance} > w((u, v)) + u.\text{distance})$ 
         $v.\text{distance} \leftarrow w((u, v)) + u.\text{distance}$ ;
  }
}
```

Minimum Spanning Tree (MST)

- Given an undirected graph $G = (V, E)$ with weights on the edges, a **minimum spanning tree (MST)** of G is a subset $T \subseteq E$ such that
 - T has no cycles
 - T contains all vertices in V
 - sum of the weights of all edges in T is minimum.
- Number of edges in T is number of vertices minus one
- Applications: circuit interconnection (minimizing tree **radius**), communication network (minimizing tree **diameter**), etc.



Prim's MST Algorithm

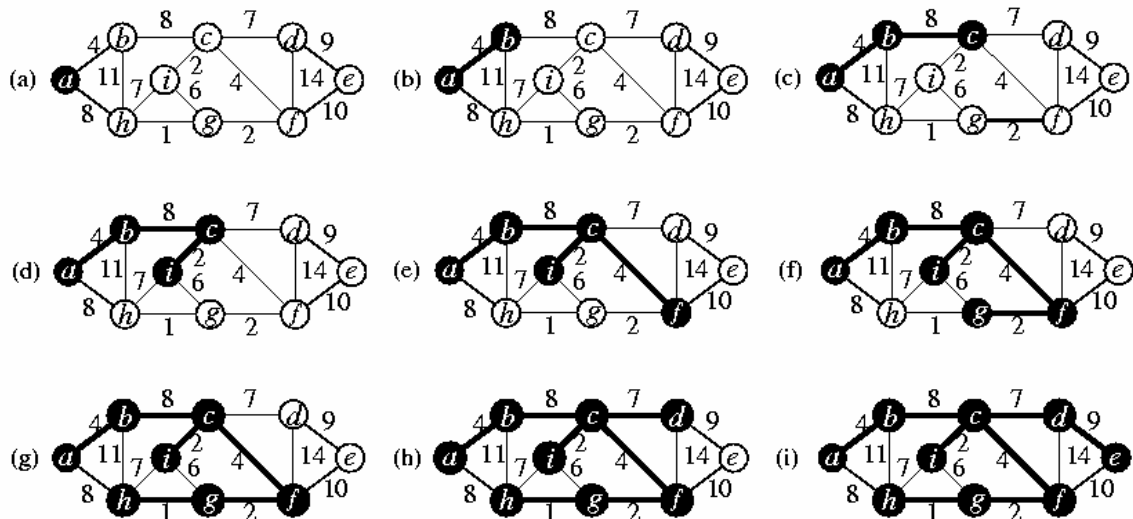
```

MST-Prim( $G, w, r$ )
1.  $Q \leftarrow V[G]$ ;
2. for each vertex  $u \in Q$ 
3.    $key[u] \leftarrow \infty$ ;
4.  $key[r] \leftarrow 0$ ;
5.  $\pi[r] \leftarrow NIL$ ;
6. while  $Q \neq \emptyset$ 
7.    $u \leftarrow \text{Extract-Minimum-Element}(Q)$ ;
8.   for each vertex  $v \in Adj[u]$ 
9.     if  $v \in Q$  and  $w(u, v) < key[v]$ 
10.       $\pi[v] \leftarrow u$ ;
11.       $key[v] \leftarrow w(u, v)$ 
    
```

- Q
priority queue for vertices not in the tree, based on $key[]$.
- $Key[]$
min weight of any edge connecting to a vertex in the tree.

- Starts from a vertex and grows until the **tree** spans all the vertices.
 - The edges in A always form a single tree.
 - At each step, a **safe, minimum-weighted** edge connecting a vertex in A to a vertex in $V - A$ is added to the tree.

Example: Prim's MST Algorithm



Time Complexity of Prim's MST Algorithm

```

MST-Prim( $G, w, r$ )
1.  $Q \leftarrow V[G]$ ;
2. for each vertex  $u \in Q$ 
3.    $key[u] \leftarrow \infty$ ;
4.    $key[r] \leftarrow 0$ ;
5.    $\pi[r] \leftarrow NIL$ ;
6. while  $Q \neq \emptyset$ 
7.    $u \leftarrow \text{Extract-Minimum-Element}(Q)$ ;
8.   for each vertex  $v \in Adj[u]$ 
9.     if  $v \in Q$  and  $w(u, v) < key[v]$ 
10.       $\pi[v] \leftarrow u$ ;
11.       $key[v] \leftarrow w(u, v)$ 
    
```

- Straightforward implementation: $O(V^2)$ time
 - Lines 1--5: $O(V)$.
 - Line 7: $O(V)$ for Extract-Minimum-Element, so $O(V^2)$ with the **while** loop.
 - Lines 8--11: $O(E)$ operations, each takes $O(\lg V)$ time.
- Run in $O(E \lg V)$ time if Q is implemented as a binary heap
- Run in $O(E + V \lg V)$ time if Q is implemented as a Fibonacci heap

Prim's MST Pseudo Code in Text

```
prim(set of struct vertex  $V$ )
{
  set of struct edge  $F$ ;
  set of struct vertex  $W$ ;
  struct vertex  $u$ ;
   $u \leftarrow$  "any vertex from  $V$ ";
   $V \leftarrow V \setminus \{u\}$ ;
   $W \leftarrow \{u\}$ ;
   $F \leftarrow \emptyset$ ;
  for each  $v \in V$ 
  if  $((u, v) \in E)$  {
     $v.distance \leftarrow w((u, v))$ ;
     $v.via\_edge \leftarrow (u, v)$ ;
  }
  else  $v.distance \leftarrow +\infty$ ;
  while  $(V \neq \emptyset)$  {
     $u \leftarrow$  " $u \in V$ , such that  $\forall v \in V : u.distance \leq v.distance$ ";
     $W \leftarrow W \cup \{u\}$ ;
     $V \leftarrow V \setminus \{u\}$ ;
     $F \leftarrow F \cup \{u.via\_edge\}$ ;
    for each  $v$  "such that  $(u, v) \in E$ "
    if  $(v.distance > w((u, v)))$  {
       $v.distance \leftarrow w((u, v))$ ;
       $v.via\_edge \leftarrow (u, v)$ ;
    }
  }
}
```