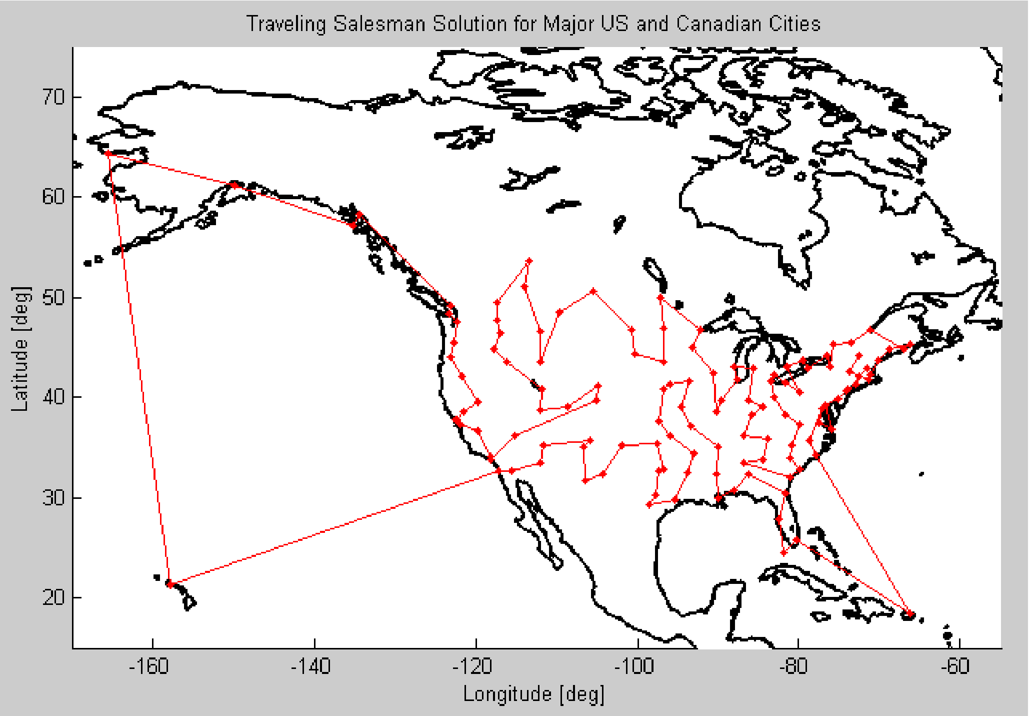
Module 11: Additional Topics
Graph Theory and Applications

Topics:

- Introduction to Graph Theory
- Representing (undirected) graphs
- Basic graph algorithms

Consider the following:

- Traveling Salesman Problem (TSP): Given N cities and the distances between them, find the shortest path to visit all cities and return to the start.

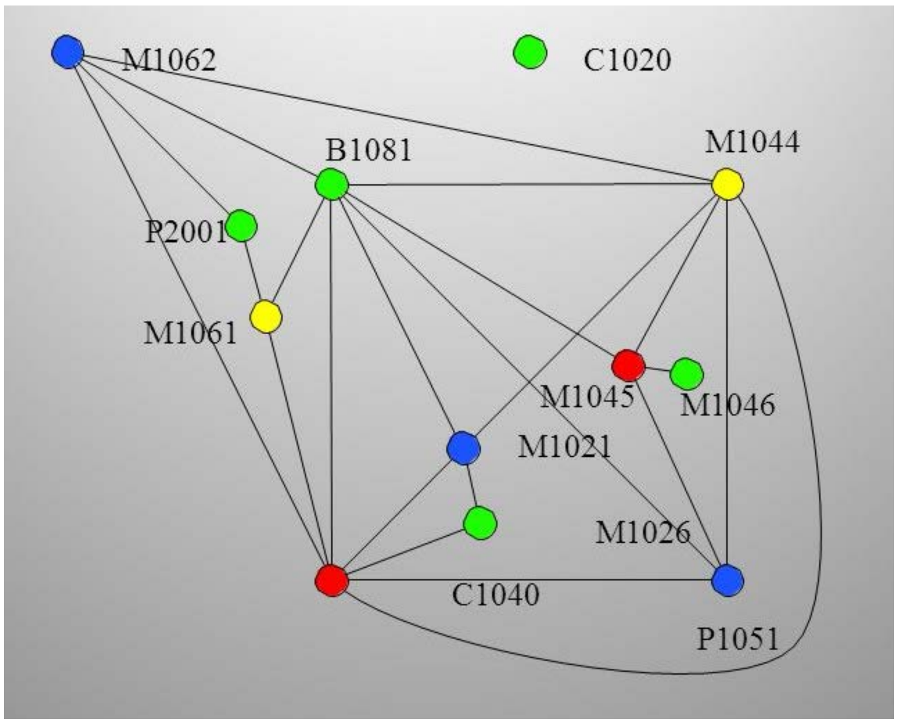


What does the TSP have in common with the following problems?

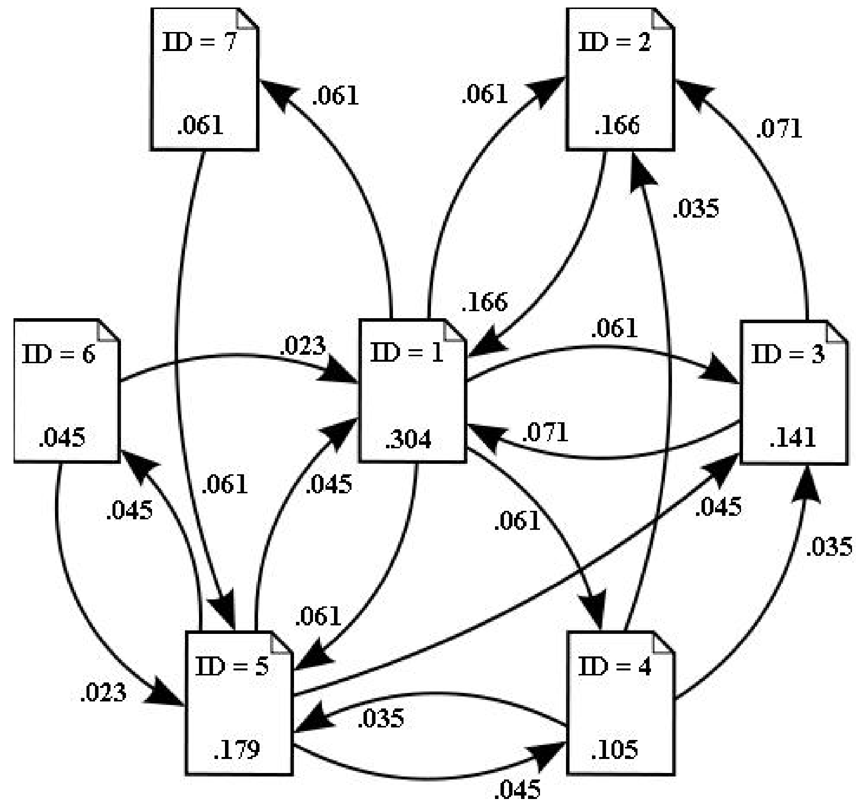
- Placement of new fire stations in a city to provide best coverage to all residents
- Ranking of "importance" of web pages by Google's PageRank algorithm
- Scheduling of final exams so they do not conflict
- Arranging components on a computer chip
- Analyzing strands of DNA
- Binary Search Trees

They all fall within the field of *GRAPH THEORY*

Non-conflicting exams

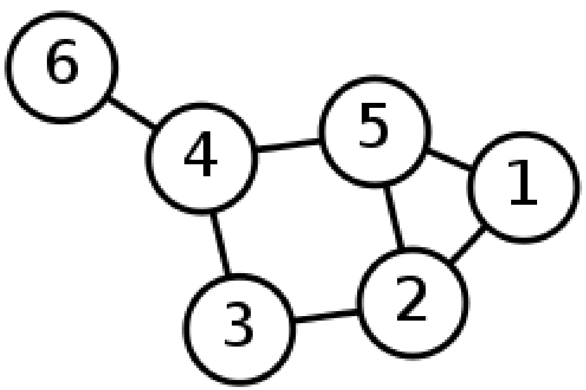


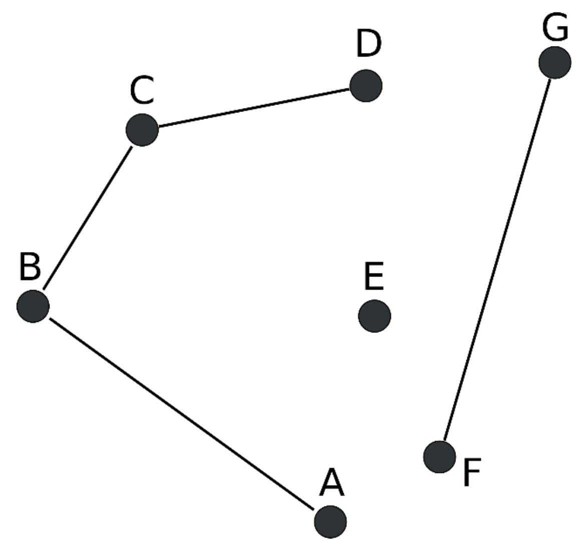
PageRank Algorithm



Undirected Simple Graphs

An undirected simple ***graph*** G is a set V, of ***vertices***, and a set E, of unordered distinct pairs from V, called ***edges***. We write G=(V,E).





Graph Terminology

- If (v_k, v_p) is an edge, we say that v_k and v_p are ***neighbours,*** and are ***adjacent.*** Note that k and p must be different.
- The number of neighbours of a vertex is also called its ***degree***
- A sequence of nodes $v_1, v_2, \ldots, v_k$ is a ***path*** of length k-1 if (v_1, v_2),(v_2, v_3),…,(v_{k-1}, v_k) are all edges
  - If $v_1 = v_k$, this is called a ***cycle***
- A graph G is ***connected*** if there exists a path through all vertices in G

Interesting Results on Graphs

Let n = number of vertices,

and m = number of edges:

1. $m \leq n(n-1)/2$
2. The number of graphs on n vertices is $2^{n(n-1)/2}$
3. The sum of the degrees over all vertices is $2m$.

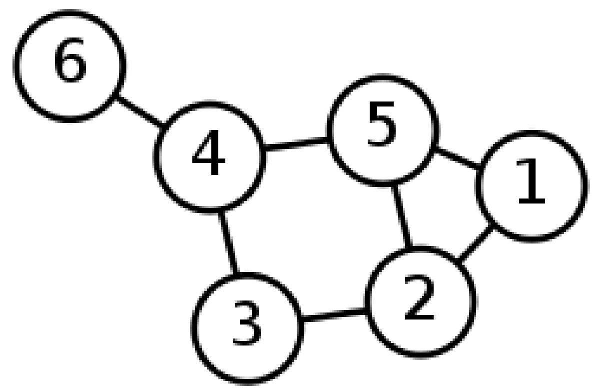
How can we store information about graphs in Python?

- We need to store labels for the vertices
  - These could be strings or integers
- We need to store both endpoints using the labels on the vertices.

- We will consider three different implementations for undirected, unweighted graphs

Implementation 1: Vertex and Edge Lists

- $\mathrm{V} = [v_1, v_2, v_3, \dots, v_m]$,
- $E = [e_1, e_2, e_3, \dots, e_m]$, where edge $e_j = [a, b]$ when vertices a and b are connected by an edge



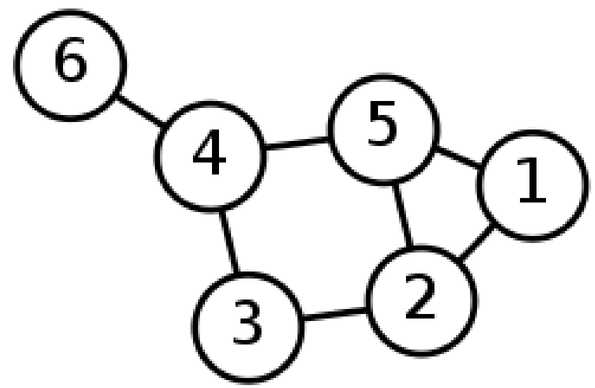

```
V=[6,4,5,3,2,1]
E=[[6,4], [4,5], [4,3], [3,2],
      [5,2], [1,2], [5,1]]
```

Implementation 2: Adjacency list

- For each vertex:
  - Store the labels on its neighbours in a list
- We will use a dictionary
  - Keys: labels of vertices
    - Recall: integers or strings can be keys
  - Associated values: List of neighbours (adjacent vertices)

Example:

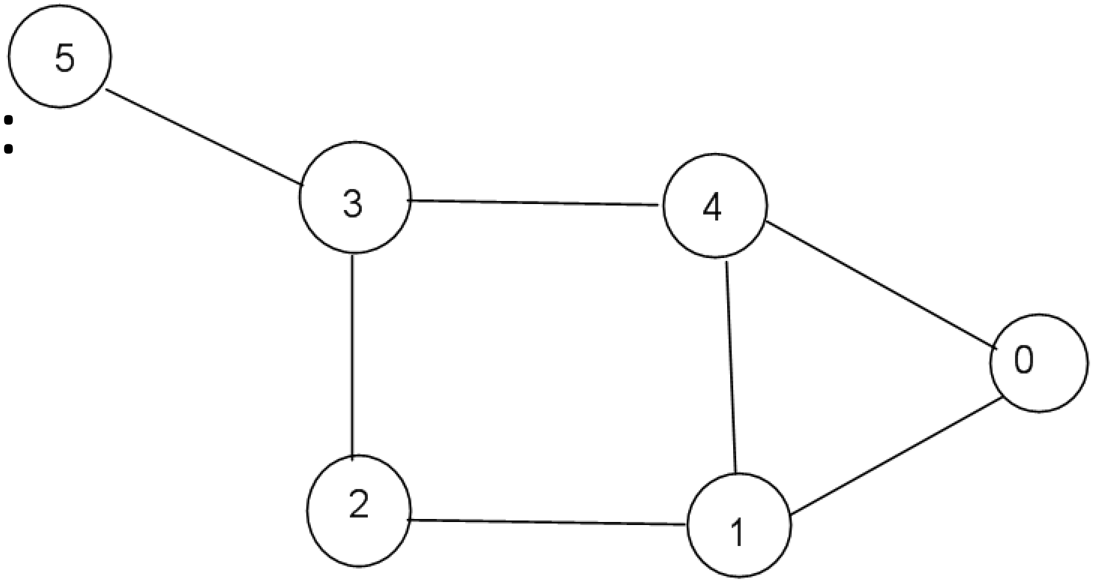
```
{1:[2,5],
 2:[1,3,5],
 3:[2,4],
 4:[3,5,6],
 5:[1,2,4],
 6:[4]}
```



Implementation 3: Adjacency Matrix

- For simplicity, assume vertices are labelled $0, \ldots, n-1$
- Create an nxn matrix for `G`
- If there is an edge connecting i and j:
  - Set `G[i][j] = 1`,
  - Set `G[j][i] = 1`
- Otherwise, set these values to 0

Example:



G:

vertex	*0*	*1*	*2*	*3*	*4*	*5*
0	[[0,	1,	0,	0,	1,	0],
1	[1,	0,	1,	0,	1,	0],
2	[0,	1,	0,	1,	0,	0],
3	[0,	0,	1,	0,	1,	1],
4	[1,	1,	0,	1,	0,	0],
5	[0,	0,	0,	1,	0,	0]]

Comparing the implementations on simple tasks

- Determine if two vertices are neighbours.
- Find all the neighbours of a vertex.

Which implementation to use?

- We'll use the adjacency list (a good case could also be made for the adjacency matrix).

Graph Traversals

- Determine all vertices of G that can be reached from a starting vertex
- There can be different types of traversals
- If you find all vertices starting from v, the graph is ***connected***
- If not all vertices can be reached, a ***connected component*** containing v has been found
- Must determine a way to ensure we do not cycle indefinitely

Applications of traversals

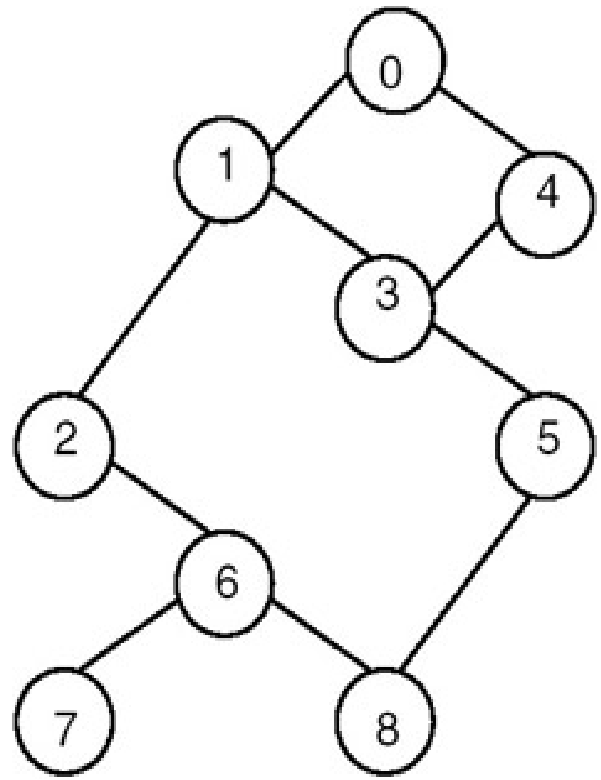
- Finding path between two vertices
- Finding connected components
- Tracing garbage collection in programs (managing memory)
- Shortest path between two points
- Planarity testing
- Solving puzzles like mazes
- Graph colouring

One approach: Breadth-first search Traversal (bfs)

- Choose a starting point v
- Visit all the neighbours of v
- Then, visit all of the neighbours of the neighbours of v, etc.
- Repeat until all reachable vertices are visited
- Need some way to avoid visiting edges more than once
- Note: there may be more than one bfs ordering of a graph, starting from v.

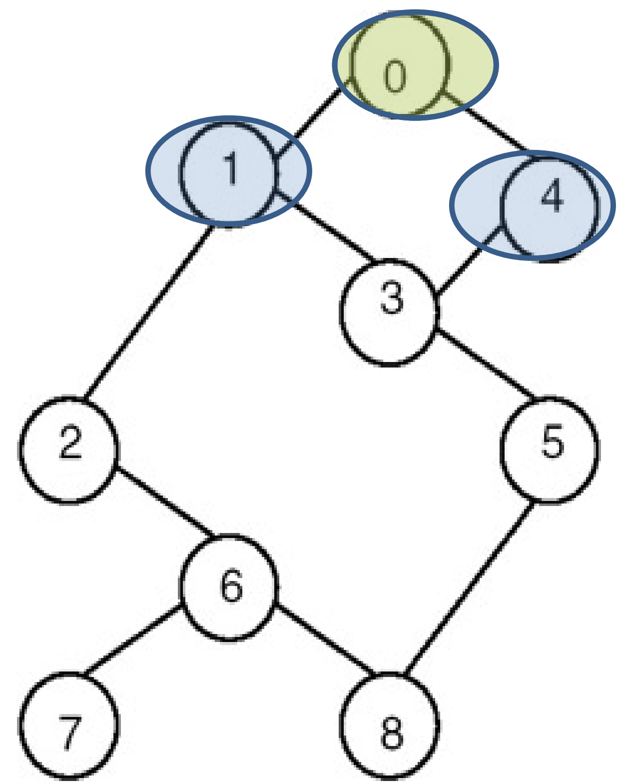
Implementation of bfs traversal

```
def bfs(graph, v):
  all = []
  Q = []
  Q.append(v)
  while Q != []:
    v = Q.pop(0)
    all.append(v)
    for n in graph[v]:
      if n not in Q and\
         n not in all:
         Q.append(n)
  return all
```



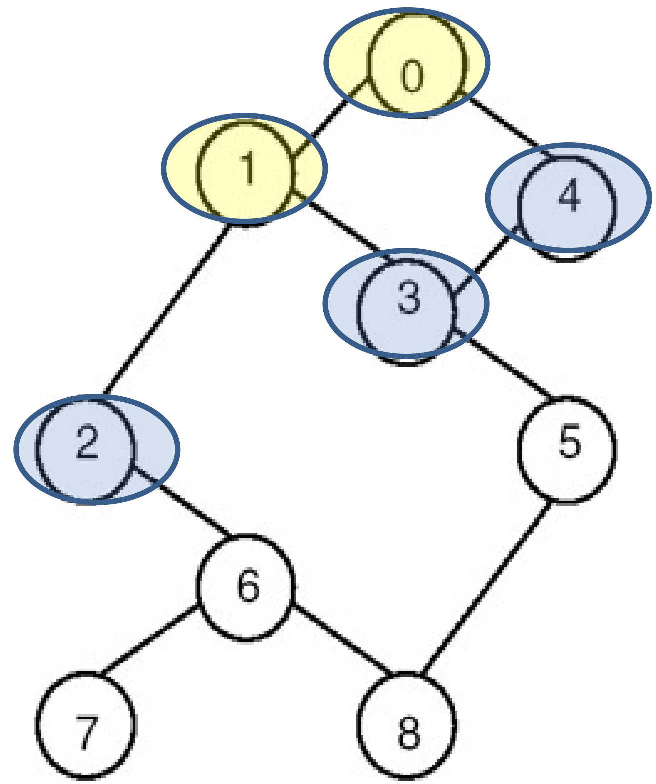
Starting bfs from 0 (1)

- Start from v=0
- all = []
- Q = [0]
  - v = 0
  - all = [0]
  - Neighbours of 0: 1,4
    - Q = [1,4]



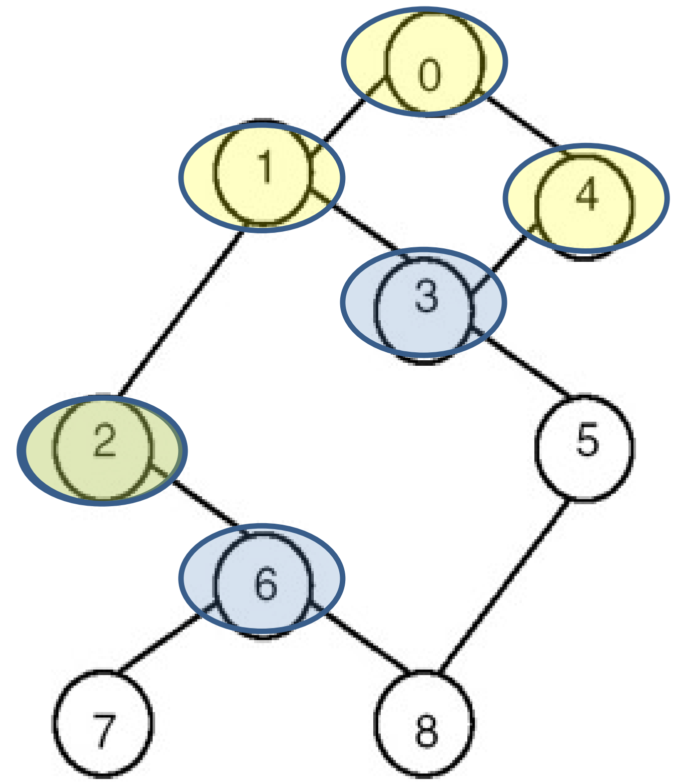
Continuing bfs (2)

- Q = [1, 4]
- v = 1
- all = [0,1]
- Neighbours of 1: 0,2,3
  - Q = [4,2,3]



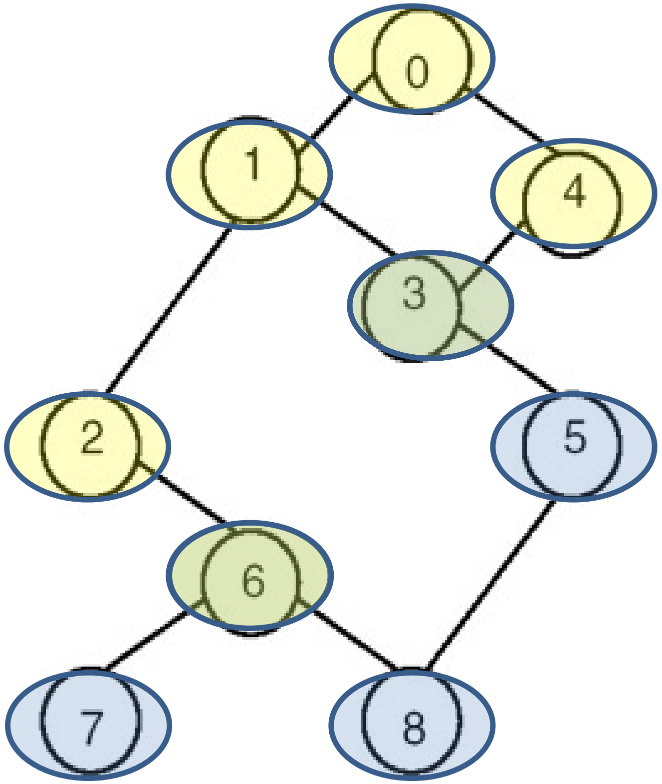
Continuing bfs (3)

- Q: [4, 2, 3]
- v = 4
- all = [0,1,4]
- Neighbours of 4: 0,3
  - No vertices added to Q
- Q= [2,3]
- v = 2
- all = [0,1,4,2]
- Neighbours of 2: 1,6 → Q = [3,6]



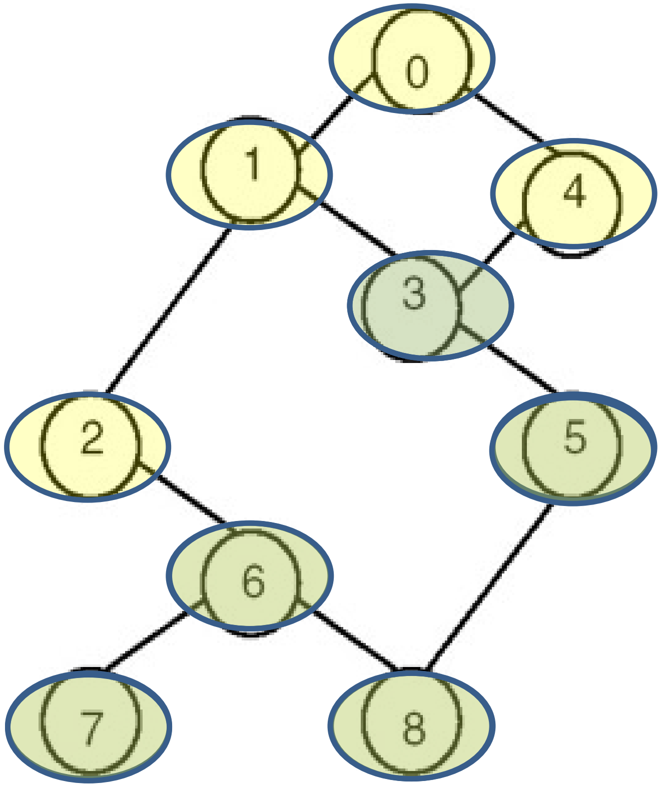
Continuing bfs (4)

- Q: [3, 6]
- v = 3
- all = [0,1,4,2,3]
- Neighbours of 3: 1,4,5
  - Q = [6,5]
- Q = [6, 5]
- v = 6
- all = [0,1,4,2,3,6]
- Neighbours of 6: 2,7,8
  - Q = [5,7,8]



Continuing bfs (5)

- Q: [5, 7, 8]
- v = 5
- all = [0,1,4,2,3,6,5]
- Neighbours of 5: 3,8 (Q unchanged)
- Q = [7,8]
- v = 7
- all = [0,1,4,2,3,6,5,7]
- Neighbours of 7: 6 (Q unchanged)
- Q = [8]
- v = 8
- all = [0,1,4,2,3,6,5,7,8]
- Neighbours of 8: 5,6 (Q unchanged)
- Q is empty

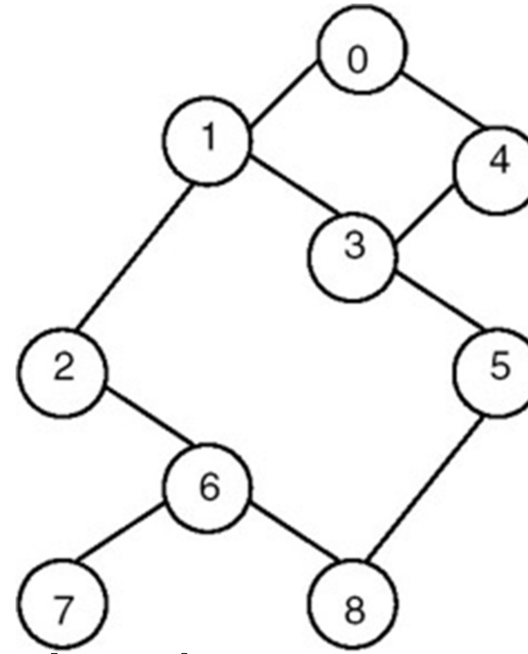


Another approach: depth-first traversal (dfs)

- Choose a starting point v
- Proceed along a path from v as far as possible
- Then, backup to previous (most recently visited) vertex, and visit its unvisited neighbour (this is called *backtracking*)
  - Repeat while unvisited, reachable vertices remain
- Note: there may be more than one dfs ordering of a graph, starting from v.

A depth first search traversal solution

```
def dfs(graph, v):
    visited = []
    S = [v]
    while S != []:
        v = S.pop()
        if v not in visited:
            visited.append(v)
            for w in graph[v]:
                if w not in visited:
                    S.append(w)
    return visited
```

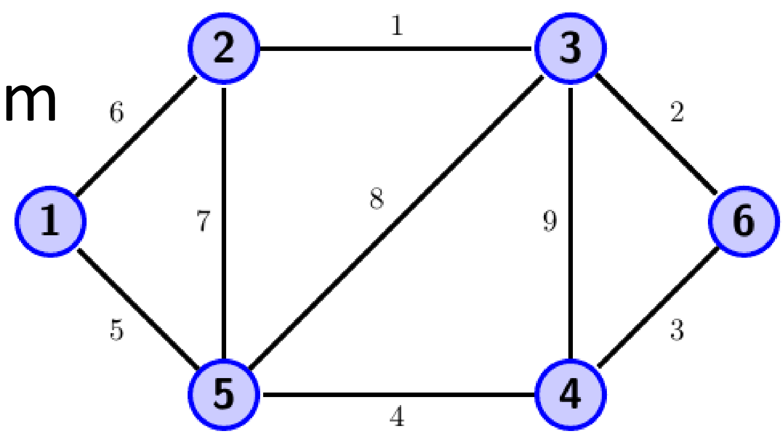


Breadth first vs depth first Searches

- Both need an additional list to store needed information:
  – BFS uses Q:
    - Add to the end and remove from the front
    - Called a Queue
  – DFS uses S:
    - Add to the end and remove from the end
    - Called a Stack
  – Stacks and Queues are both very useful in CS

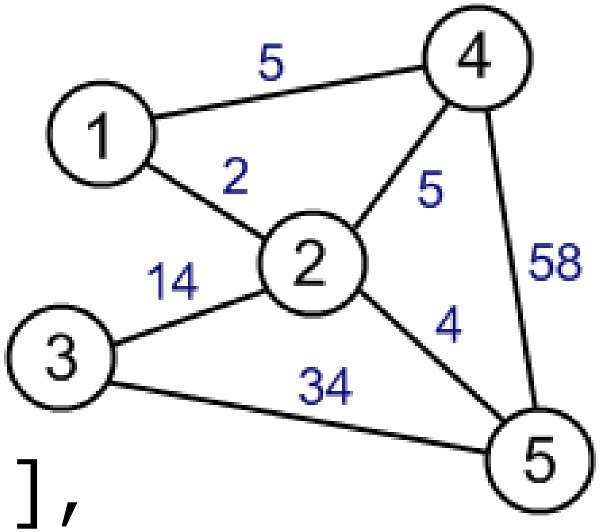
Weighted edges

- Each edge has an associated weight. It might represent:
  - Distance between cities
  - Cost to move between locations
  - Capacity of a route
  - Probability of moving from one web page to another



Adjust adjacency list to include weights

- Adjust our adjacency list to store weights with each edge
- ```
  {1:[[2,2],[4,5]],
    2:[[1,2],[3,14],
       [4,5],[5,4]],
    3:[[2,14],[5,34]],
    4:[[1,5],[2,5],[5,58]],
    5:[[2,4],[3,34],[4,58]]}
  ```


  ```

Shortest Paths Problem

Problem: Given a weighted graph, G, and vertex ***s*** (called the source), find the path of least weight from ***s*** to each of the other vertices in the graph.

The total ***weight of a path*** is the sum of the weights of all its edges.

Assumptions:

- Weights are all positive
- There exists at least one path from ***s*** to each vertex

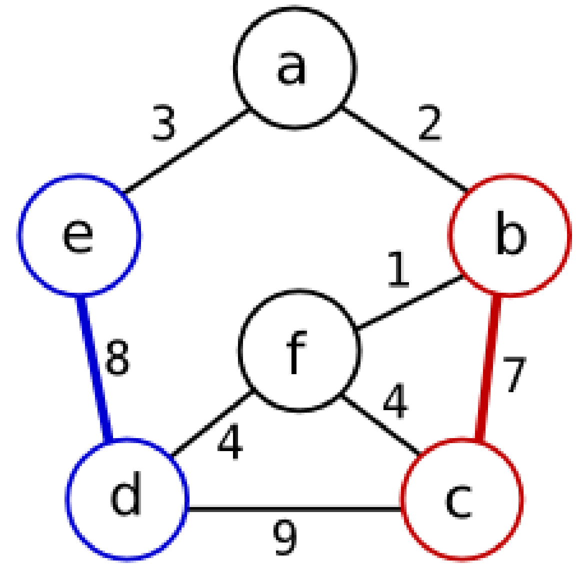
Dijkstra's Algorithm for the Shortest Paths Problem

- Famous algorithm in CS
- Example of a ***Greedy Algorithm***
  - At each step, the locally optimum choice is made in hopes of finding the global optimum.

Example of Dijkstra's Algorithm (1)

- Find shortest paths from: ***a***
- Keep track of the vertices

that you know the shortest path for, ***S = [a]*** to start



- For all vertices, determine

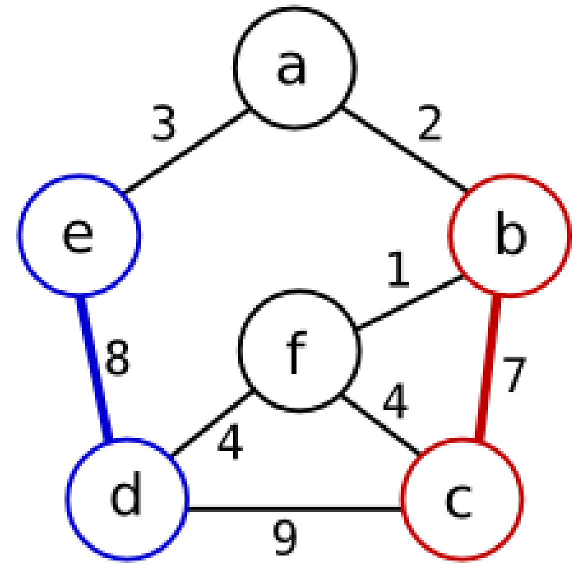
the weight of the path from ***a*** using only vertices in ***S***. Note that some vertices are not reachable yet.

Continuing Dijkstra's Algorithm (2)

***S* = [*a*]**

D: Distances through S

a	*b*	*c*	*d*	*e*	*f*
0	*2*	∞	∞	*3*	∞



Greedy: Choose the vertex with the minimum positive distance from ***a*** through *S*: ***b***

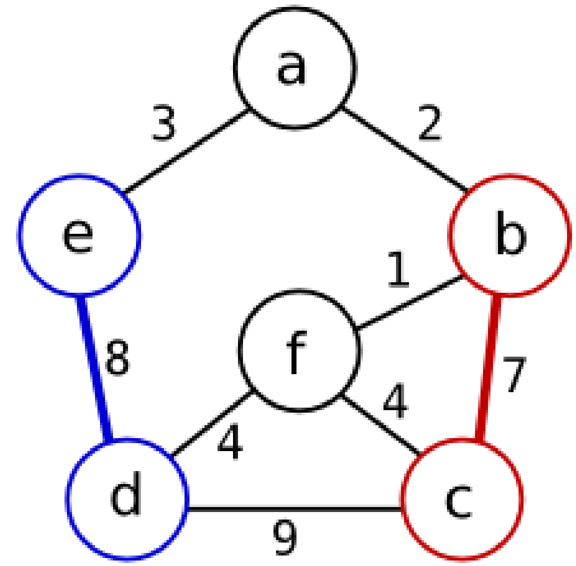
Add *b* to *S*

Continuing Dijkstra's Algorithm (3)

***S* = [*a*,*b*]**

D: Distances through *S*

a	*b*	*c*	*d*	*e*	*f*
0	***2***	*9*	∞	*3*	*3*



Greedy: Choose the vertex with the minimum positive distance from a through *S*: ***e*** and ***f***

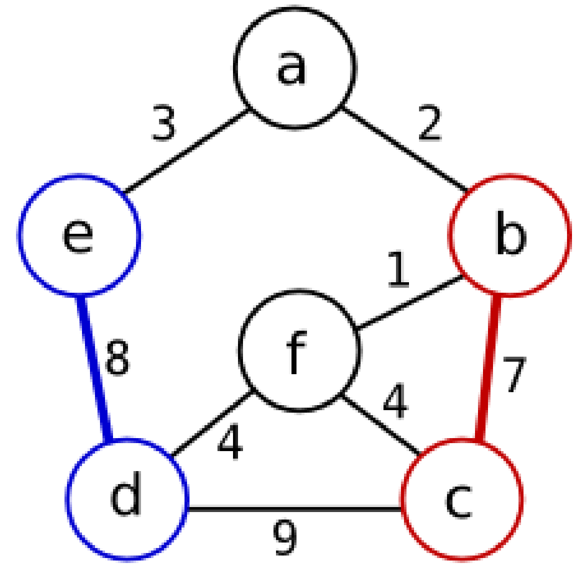
Add ***e*** to *S* (random choice)

Continuing Dijkstra's Algorithm (4)

***S* = [*a*,*b*,*e*]**

D: Distances through *S*

a	*b*	*c*	*d*	*e*	*f*
0	***2***	*9*	*11*	***3***	*3*



Greedy: Choose the vertex with the minimum positive distance from a through *S*: ***f***

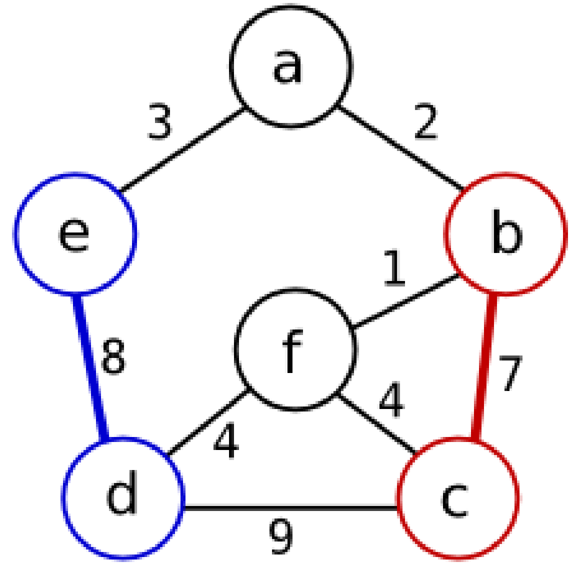
Add ***f*** to *S*

Continuing Dijkstra's Algorithm (5)

***S* = [*a*,*b*,*e*,*f*]**

D: Distances through *S*

a	***b***	***c***	***d***	***e***	***f***
0	***2***	*7*	*7*	***3***	***3***



Greedy: Choose the vertex with the minimum positive distance from a through *S: **c** and **d***

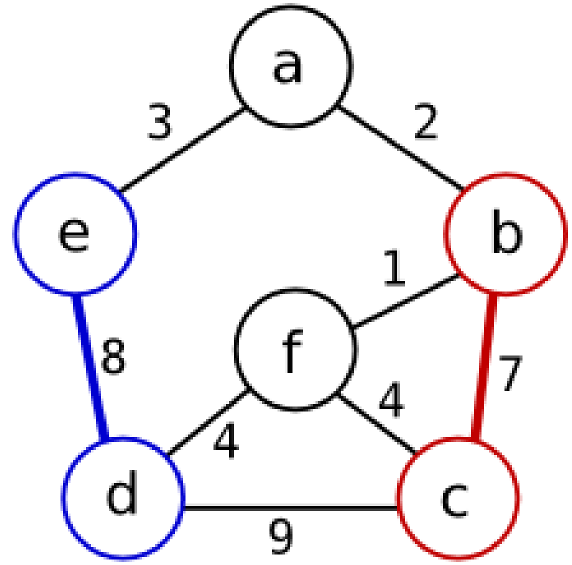
Add ***d*** to *S (random choice)*

Continuing Dijkstra's Algorithm (6)

***S* = [*a*,*b*,*e*,*f*,*d*]**

D: Distances through *S*

a	***b***	***c***	***d***	***e***	***f***
0	***2***	*7*	***7***	***3***	***3***



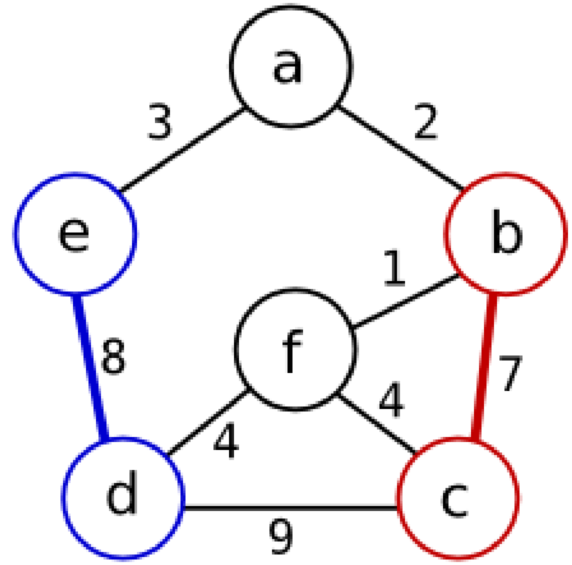
Greedy: Choose the vertex with the minimum positive distance from a through *S*: ***c***

Add ***c*** to *S*

Continuing Dijkstra's Algorithm (7)

Length of shortest path from ***a*** to each of the vertices:

a	*b*	*c*	*d*	*e*	*f*
0	*2*	*7*	*7*	*3*	*3*



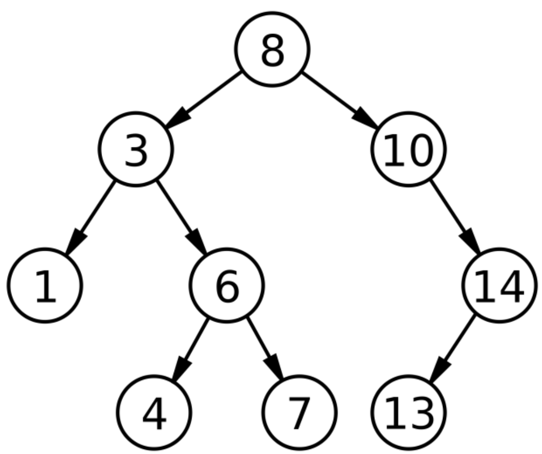
Note: Can modify basic Dijkstra's algorithm to keep track of edges used in shortest paths.

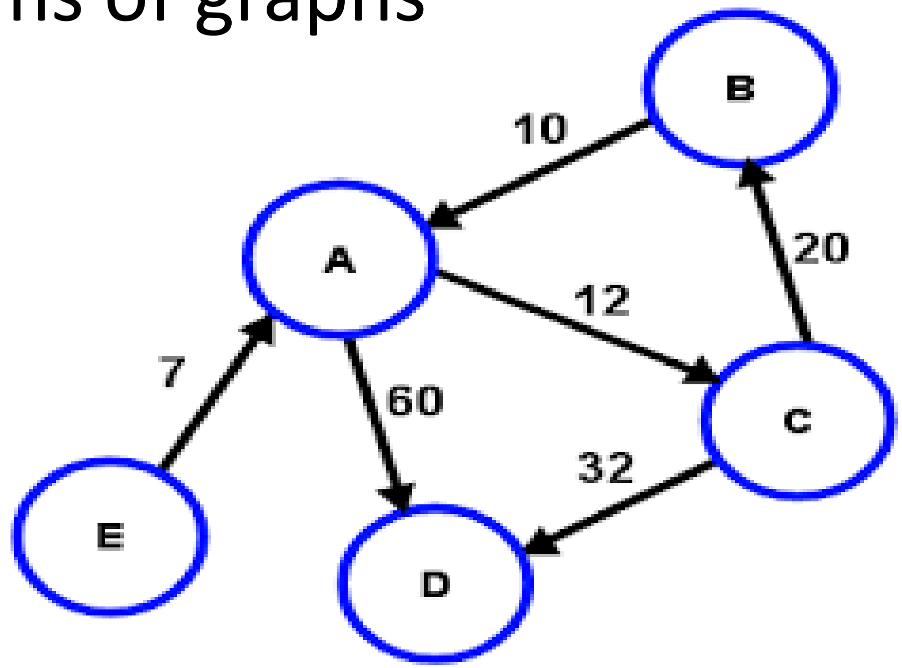
More on Greedy algorithms

- Often used to solve very difficult problems (like the Travelling Salesman problem).
- Depending on the problem, may not always provide an optimal solution.
  - Often acceptable if all known algorithms for an optimal solution have exponential runtime

Other types of graphs

- Edges can be directed – from one vertex to another
- Directed edges can have weights as well
- Trees are special forms of graphs





Goals of Module 11

- Understand basic graph terminology
- Understand representation of graphs in Python
- Understand breadth-first and depth-first search traversals
- Understand Dijkstra's algorithm