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 \((v_1, v_2), (v_2, v_3), \ldots, (v_{k-1}, v_k)\) 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

- $V = [v_1, v_2, v_3, ..., v_m]$
- $E = [e_1, e_2, e_3, ..., e_m]$, 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, ..., \(n - 1\)
• Create an \(n \times n\) 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:

<table>
<thead>
<tr>
<th>vertex</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>[0, 1, 0, 0, 1, 0]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>[1, 0, 1, 0, 1, 0]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>[0, 1, 0, 1, 0, 0]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>[0, 0, 1, 0, 1, 1]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>[1, 1, 0, 1, 0, 0]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>[0, 0, 0, 1, 0, 0]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Graph representation with vertices and adjacency matrix.
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

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
<th>e</th>
<th>f</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>0</td>
<td>2</td>
<td>∞</td>
<td>∞</td>
<td>3</td>
<td>∞</td>
</tr>
</tbody>
</table>

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 \( S \)

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>b</td>
<td>c</td>
<td>d</td>
<td>e</td>
<td>f</td>
</tr>
<tr>
<td>0</td>
<td>2</td>
<td>9</td>
<td>( \infty )</td>
<td>3</td>
<td>3</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
<th>e</th>
<th>f</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2</td>
<td>9</td>
<td>11</td>
<td>3</td>
<td>3</td>
</tr>
</tbody>
</table>

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 $S$

<table>
<thead>
<tr>
<th></th>
<th>$a$</th>
<th>$b$</th>
<th>$c$</th>
<th>$d$</th>
<th>$e$</th>
<th>$f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0$</td>
<td>$2$</td>
<td>$7$</td>
<td>$7$</td>
<td>$3$</td>
<td>$3$</td>
<td></td>
</tr>
</tbody>
</table>

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

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>b</td>
<td>c</td>
<td>d</td>
<td>e</td>
<td>f</td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>0</td>
<td>2</td>
<td>7</td>
<td>7</td>
<td>3</td>
<td>3</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
<th>e</th>
<th>f</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2</td>
<td>7</td>
<td>7</td>
<td>3</td>
<td>3</td>
<td>3</td>
</tr>
</tbody>
</table>

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