Scientific Computation

Spring, **2019**

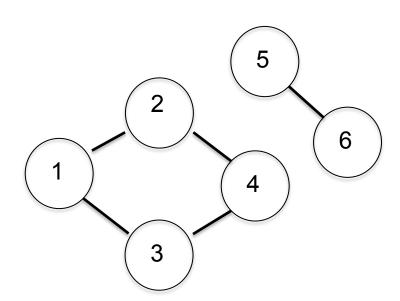
Lecture 8

Today

- Depth-first search
- Dijkstra's algorithm for weighted networks

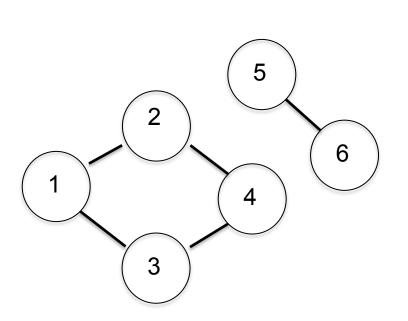
Graph search

- Basic idea: Given a graph, G, and a source node, s, find all other nodes that can be reached from s
- Basic approach:
 - Label s as "explored" and all other nodes as "unexplored"
 While there is at least one edge between an explored and unexplored node:
 Select one such edge and re-label the unexplored node as explored



Graph search

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Implementation: Depends on how edges are selected each iteration

- Depth-first search aggressively move into the graph (1-2, 2-4)
- Breadth-first search consider one "layer" at a time (1-2, 1-3)
- Today: DFS

Breadth-first search

- Python implementation
 - Specify: Graph and source node
 - Maintain: 1) list of nodes, 2) list of labels for nodes and 3) queue of nodes to-be explored
 - Initialize the queue with the source node and mark it as explored
 - Remove nodes from the queue in the order they were added (first in, first out)
 - Search through edges of removed node and add unexplored nodes to queue
 - Label added nodes as explored
 - Terminate search when queue is empty

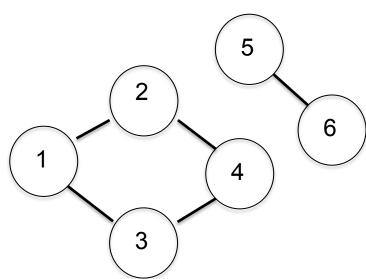
Breadth-first search

Specify: Graph and source node

```
G = nx.Graph()
edges = [[1,2],[1,3],[1,2],[2,4],[3,4],[5,6]]
G.add_edges_from(edges)
s = 1
Q = [s] #Nodes to be explored
```

Create list of nodes and labels

```
a_list = G.adjacency_list()
nodes = G.nodes()
z = [0 for i in nodes] #labels
L = [nodes,z]
L[1][s-1]=1 #mark source node as explored
```



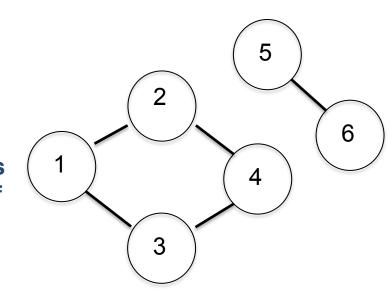
Iterate through nodes in queue (updating Q as appropriate)

```
while len(Q)>0:
    n = Q.pop(0)
    for v in a_list[n-1]: #iterate through neighbors of n
        if L[1][v-1]==0:
            L[1][v-1]=1
            Q.append(v)
```

Breadth-first search

Adding print("n=%d,Q=" %(n),Q) to the while loop and running the code:

• n is the node removed from the queue and Q is the queue after edges from n have been added (if n is unexplored



Depth-first search

6

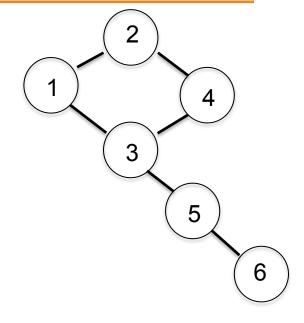
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- What changes for DFS?
- How much does the code change?
- The problem setup and initialization will be the same
- Can focus on the search through the graph
- BFS: Remove node from front of queue, append unexplored neighbors to back of queue
- DFS: Remove node from end of stack, append unexplored neighbors to end of stack

```
#Depth-first search
while len(Q)>0:
    n = Q.pop() #Only change from BFS
    for v in a_list[n-1]: #iterate through neighbors of n
        if L[1][v-1]==0:
        L[1][v-1]=1
        Q.append(v)
```

Depth-first search

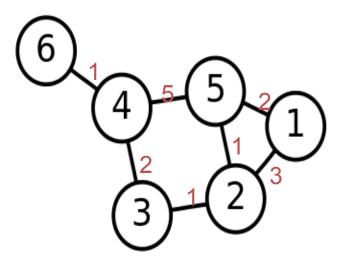
- Let's compare DFS and BFS on this modified graph
- Output from codes is provided below
- Compare the order in which the nodes are visited



 We have left the length calculation in the DFS code the same as in BFS – is this correct?

Weighted networks

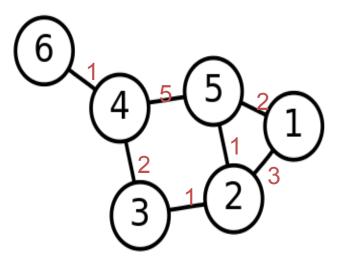
- Have considered unweighted networks so far
- Often have a weight associated with each edge
 - E.g. distance between nodes, time to travel between nodes
 - More generally, nodes can represent states in a state space, and weights can represent the cost of moving between states
- What is the best way to compute shortest paths in a weighted network?
- Can we use BFS or DFS? If weights are small, can replace a weight-n link with n weight-1 links
 - But weights can be arbitrarily large
- Dijkstra's algorithm is a graph-search method for networks with positive weights



Shortest paths:

1→2: 3

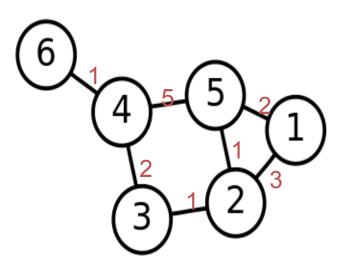
- Dijkstra's algorithm is a graph-search method for networks with positive weights
- Input: Graph (nodes, edges, weights) and source node
- Output: Shortest paths from source node to all nodes reachable from source



Shortest paths:

1→2: 3

- Dijkstra's algorithm is a graph-search method for networks with positive weights
- Input: Graph (nodes, edges, weights) and source node
- Output: Shortest paths from source node to all nodes reachable from source
- Basic idea:
 - Maintain lists of explored and unexplored nodes (E and U)
 - For each explored node, assume that we have calculated the shortest distance to the source
 - Each iteration, move one node from U to E
 - Which node? The neighbor of an explored node that is closest to the source.

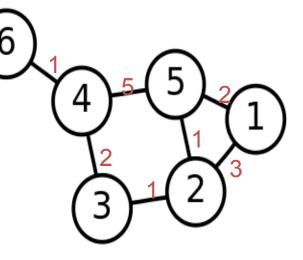


Shortest paths:

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Basic idea:

- Maintain lists of explored and unexplored nodes (E and U)
- For each explored node, assume that we have calculated the shortest distance to the source
- Each iteration, move one node from U to E
 - Which node? The neighbor of an explored node that is closest to the source, s
- Why is this the right node to move?
 - Let w_{ij} be the weight of the edge between nodes i and j
 - Let d_i be the length of the shortest path between node i and the source, s
 - Then d_i+w_{ij} is the length of the path between the source and node j which includes edge i,j
 - If we choose the "unexplored neighbor" with the minimum value of (d_i+w_{ij}), then all other paths from s to j will be longer (why?)

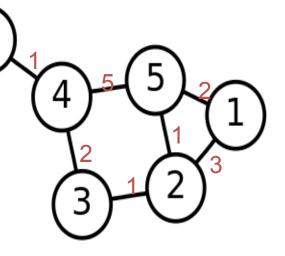


Shortest paths:

1→2: 3

Algorithm (sketch)

- 1) Set the distance for the source to be zero
- 2) Set the distances for all other nodes to an arbitrary large number (much larger than the expected largest path lengths)
- 3) Label source as explored
- 4) Set provisional distances for all neighbors of s with weights of edges between s and neighbors
- 5) Each iteration, find the unexplored node (node i) that is closest to the source (smallest provisional distance)
- 6) Label this node as explored
- 7) Update the provisional distance of all neighbors of i with min(d_i,d_i+w_{ii})
- 8) Continue "exploring" until no reachable nodes remain Imperial College unexplored.

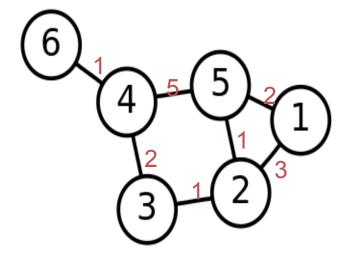


Shortest paths:

1→2: 3

Python implementation

- What data type(s) should we use?
 - list, array, dictionary, something else?
- Basic operations needed:
 - find min
 - insert/delete
- Let's try dictionaries

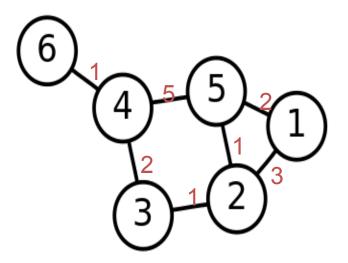


Shortest paths:

1→2: 3

Python implementation

- What data type(s) should we use?
 - list, array, dictionary, something else?
- Basic operations needed:
 - find min
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- Let's try dictionaries
- We'll work with two dictionaries one for explored nodes (where the shortest path length has been determined) and one for unexplored neighbors of explored nodes (where provisional shortest paths have been specified)
- And we'll also have the adjacency list of the graph containing the edges and their weights



Shortest paths:

1→2: 3

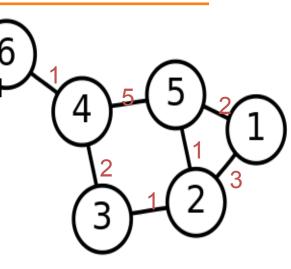
 $1 \rightarrow 4:6$

Python implementation

1. Create the graph, initialize the dicts

```
e=[[1,2,3],[1,5,2],[2,5,1],[2,3,1],[3,4,2],[4,5,5],[4,6,1]]
G = nx.Graph()
G.add_weighted_edges_from(e)

Udict = {} #Unexplored neighbor nodes
Udict[5]=0
Edict={} #Explored nodes
```



Shortest paths:

1→2: 3

Python implementation

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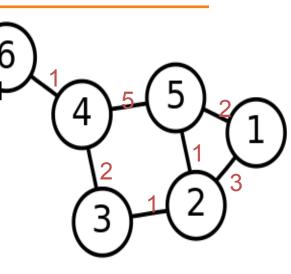
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Udict[5]=0
Edict={} #Explored nodes
```

2. Find node in Udict with smallest distance

```
while len(Udict)>0:
    dmin=2000000
    for k,v in Udict.items():
        if v<dmin:
            dmin=v #min distance
            n=k #corresponding node</pre>
```

3. Remove 'smallest-distance' node and update provisional distances of its neighbors



Shortest paths:

1→2: 3

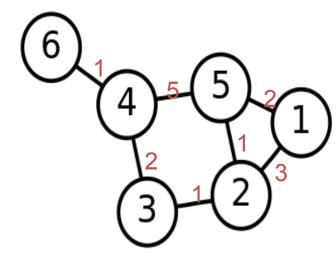
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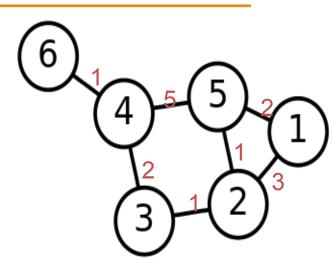
Shortest paths:

1→2: 3

Setting the source to be node 5 and running the code:

```
In [56]: Edict
Out[56]: {1: 2, 2: 1, 3: 2, 4: 4, 5: 0, 6: 5}
```

The key-value pairs are node:distance



What is the cost for a graph with N nodes and M edges?

- Estimate cost of setting up graph to be O(N+M)
- Each edge is only considered maximum of two times → O(M)
- dmin calculation → O(N²) operations
- So it is the minimum calculation which is the bottleneck
- Can we do better?

