Graphs Lecture

03/21/2016

Morning Goals

- General understanding of graphs
- How to traverse a graph
- Importance of a node through various measures of centrality

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What is a Graph?

A Graph is an ordered pair $G = (V, E)$ such that V is a set of **verticies** and E is a set of **edges** or relations. Each edge is a two element subset of V.

If an edge exists between two nodes v_i and v_j (i.e. $\{v_i, v_j\} \in E$), we say those nodes are *connected*.

Terminology

- **Node / Vertex**: A node or vertex is a single point in a graph
- **Neighbors**: The *neighbors* of a node are the nodes that it is connected to.
- **Degree**: The *degree* of a node is the number of neighbors a node has. In the case of a directed graph, the degree of a node is split into indegree and outdegree.
- **Walk**: A *walk* is a sequence of nodes and edges that connect them. A walk is said to be *open* if the starting and ending nodes are different and *closed* otherwise. The *length* of the walk is the number of edges.
- **Path**: A *path* is a walk where no node is crossed twice (called a *simple* walk). A closed path is known as a *cycle*.
- **Connected**: A graph is *connected* if every pair of vertices is connected by some path (i.e. they are either directly connected by an edge(s) or there exists a walk between them)
- **Subgraph**: A *subgraph* is a subset of the nodes of a graph and all the edges between them.
- **Connected Component**: A *connected component* is a subgraph that is connected and which is connected to no additional vertices in the supergraph.
- **Graph Diameter**: The *diameter* of a graph is the largest number of vertices that much be traversed in order to get from one vertex to any other vertex.

Types of Graphs

- **Directed Graph**: A *directed graph* is a graph where edges go in one direction (e.g. following someone on Twitter)

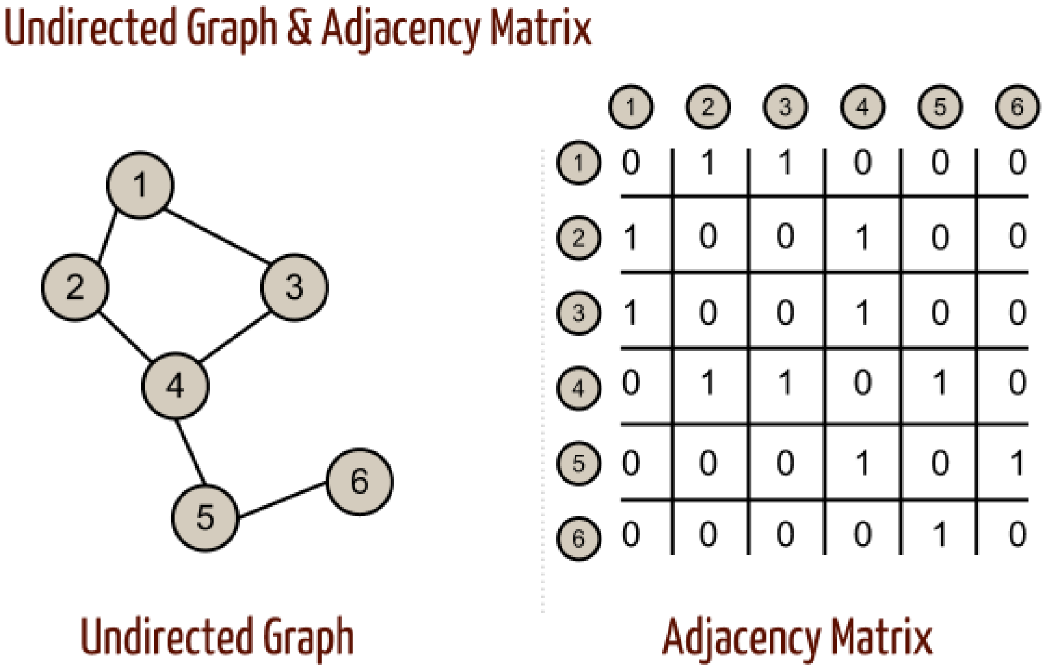
- **Undirected Graph**: A *undirected graph* is a graph where edges go in both directions (e.g. friending someone on FaceBook)
- **Weighted Graph**: In a *weighted graph* the edges have an associated weight (e.g. number of times a user retweeted another user)
- **Unweighted Graph**: In a *unweighted graph* the edges have no weight (or all edges are considered to have the same weight)
- **Bipartite**: A *bipartite graph* is a graph whose vertices can be divided into two disjoint sets such that every edge connects a vertex from one set to a vertex in the other set (e.g. a graph of actors and movies)

Data Structures

There are a variety of ways to store the components of a graph in a data structure with the most common being adjacency matrices and adjacency lists.

Adjacency Matrix

Adjacency matrices are quick to look up but suffer from the downside that they take up significant space. The majority of the values in an adjacency matrix will be zeros which take up the same amount of space as non-zero cells. Indeed, most online social networks have a *density* (the ratio of non-zero cells to zero cells) of 0.1% or less.



	1	2	3	4	5	6
1	0	1	1	0	0	0
2	1	0	0	1	0	0
3	1	0	0	1	0	0
4	0	1	1	0	1	0
5	0	0	0	1	0	1
6	0	0	0	0	1	0

Figure 1: Adjacency Matrix

Adjacency List

Adjacency lists take up significantly less space and, if implemented using the Python `dict` data structures (see below), searching, adding, and removing nodes and edges is quick and efficient.

```
edges = {'A': {'B': 2, 'D': 5, 'E': 5}, 'B': {'A': 2, 'D': 1}}
```

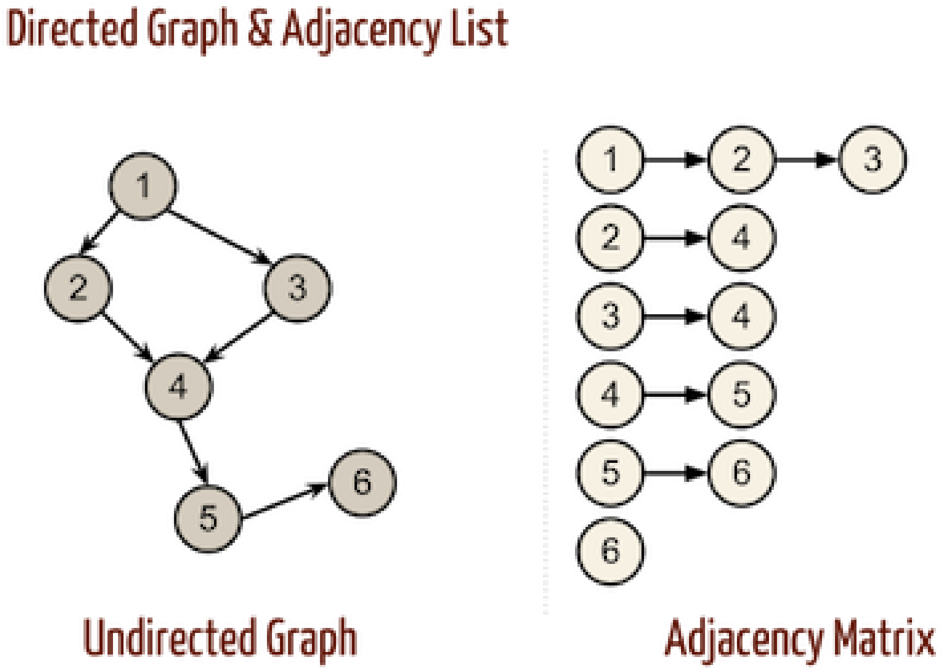


Figure 2: Adjacency List

Centrality

Measures of centrality roughly indicate the importance of a particular node. Centrality is formal way of analyzing networks to measure power and influence of each $v_i \in V$. In terms of a social network, an actors influence often only extends up to two steps away and therefore their ability to influence the overall structure of the network is directly affected by their neighbors and the neighbors of their neighbors.

Degree Centrality

- An important node is connected to a large number of other nodes
- We normalize the degree centrality by dividing by $|V| - 1$, this will make the degree centrality of a particular node be between 0 and 1
- Degree Centrality does not always capture the most "important" nodes such as those connecting different subgraphs

Closeness Centrality

Closeness Centrality involves finding the shortest path between every pair of nodes in the network using Dijkstra's algorithm and finding the average distance between any two nodes. Due to the overwhelming number of combinations of nodes in a graph, the calculation of closeness centrality is computationally expensive.

Betweenness Centrality

We can also consider a node important if it controls the passage from one node to another, or presides over a communication bottleneck in social networking terms. We quantify this with $C_b(v)$, which is the sum of fractions of shortest paths that pass through vertex v,

$$C_b(v) = \sum_{s \neq v \neq t} \frac{\sigma_{st}(v)}{\sigma_{st}}$$

where $\sigma_{st}(v)$ is the # of shortest paths between s and t that pass through v and σ_{st} is the # of shortest paths between s and t. We would then normalize this centrality using the following equation

$$normal(C_b(v)) = \frac{C_b(v)}{(N-1)(N-2)}$$

where N is the number of nodes in the graph.

Eigenvector Centrality

Eigenvector centrality, C_E, is another way of measuring whether a vector is important. This measure of centrality is able to identify so called “gray cardinals”, who may not be identified when using metrics such as degree centrality, betweenness or closeness (e.g. a mob boss who intentionally isolates himself from any direct connections to crime). It considers a vector to be important if it has important neighbors (i.e. connected to nodes with high degree) but doesn't necessarily have to have high degree itself.
Eigenvector centrality can be thought of as a recursive version of degree centrality. The algorithm works as follows:

1. Start by assigning a centrality score of 1 to all nodes ($v_i = 1, \forall v_i \in V$)
2. Recompute the scores of each node as a weighted sum of centralities of all nodes in a node's neighborhood:
$$v_i = \sum_{j \in N} x_{i,j} * v_j$$
3. Normalize v by dividing each value by the largest value.
4. Repeat steps 2 and 3 until the values of v stop changing.

This an iterative algorithm which requires iterating through all neighbors of a node to compute the weighted degree and thus is extremely computationally expensive and is thus not realistic to compute on very large networks.

Graph Traversal

In order to perform graph related operations such as determining components and shortest paths we must have a way of systematically visiting all the nodes. The most popular graph traversal algorithm is the **Breath First Search**.

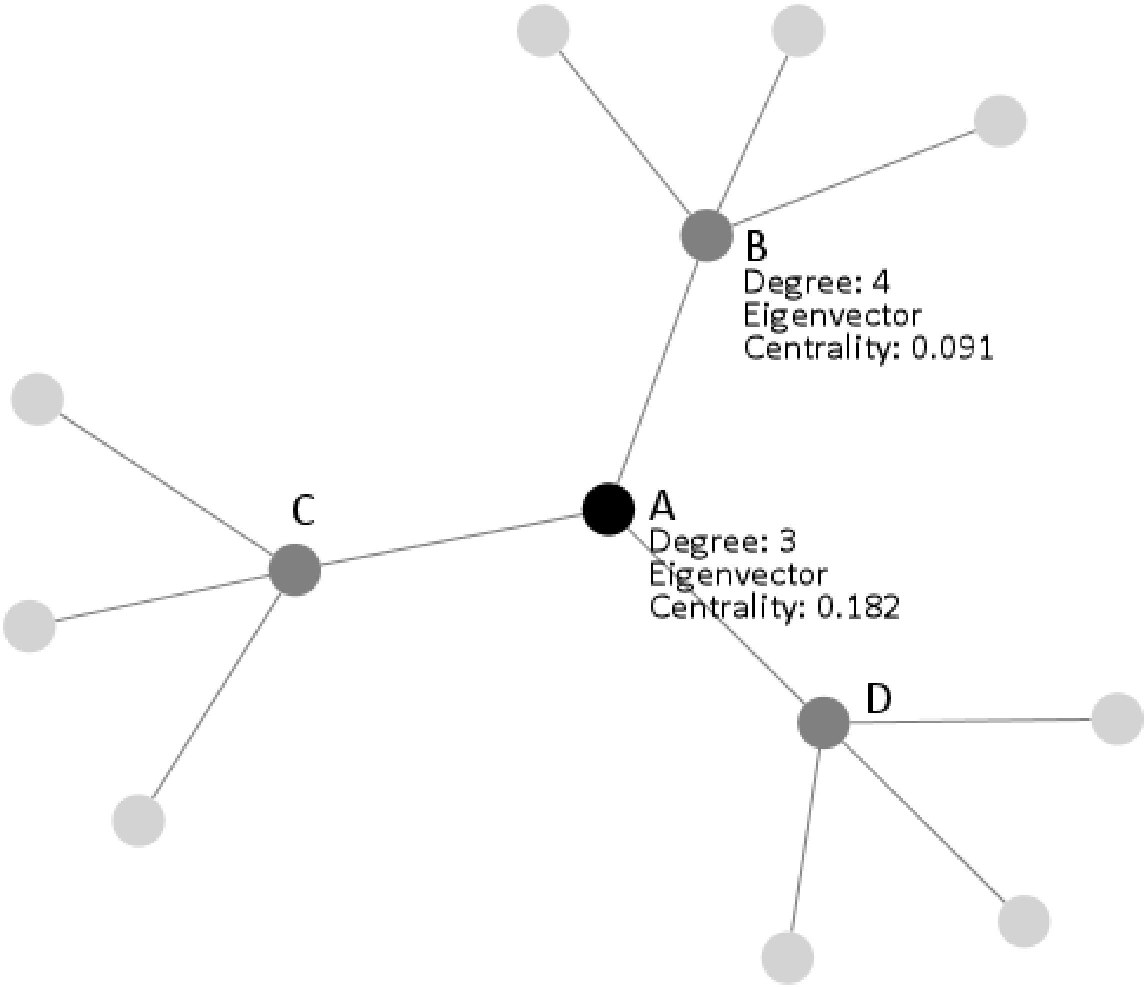


Figure 3: Example of a node with low degree, but high eigenvector centrality

Breath First Search

A Breath First Search consists of visiting all the neighbors of a node before visiting the neighbors of those neighbors. This is done by using a First In, First Out (FIFO) queue.

The following code shows how to go about implementing a breath first search utilizing the `deque` object to find all the connected components. implementing the `bfs_shortest_path_length()` and `bfs_shortest_path()` functions are left as exercises for the reader.

```
from collections import deque

def bfs_connected_components(graph, starting_node):
    '''
    Returns the connected component of a graph containing the starting_node
    '''
    visited = set()
    queue = deque([starting_node])
    while queue:
        node = queue.popleft()
        if node not in visited:
            visited.add(node)
            neighbors = graph[node]
            queue.extend(neighbors)
    return visited

if __name__ == '__main__':
    graph = {'A': {'B', 'C'},
             'B': {'A', 'E'},
             'C': {'A', 'D', 'E'},
             'D': {'C', 'E'},
             'E': {'B', 'C', 'D'}}
    starting_node = 'A'
    target_node = 'E'
    print bfs_connected_components(graph, starting_node)
    print bfs_shortest_path_length(graph, starting_node, target_node)
    print bfs_shortest_path(graph, starting_node, target_node)
```

Dijkstra’s Algorithm

Dijkstra’s Algorithm is a way of identifying the shortest path between two nodes on a weighted graph and is run with an initial node and a goal node. The resulting path will have the least cost between the two nodes.

1. Start by assigning each node a tentative distance value, setting it to zero for the initial node and infinity for all other nodes.
2. Keep a set of visited nodes which starts with just the initial node.
3. For the current node, consider all of its unvisited neighbors and calculate distance to the current node + distance from current node to the neighbor. If this is less than their current tentative distance, replace it with this new value.

4. When all neighbors have been considered, mark the current node as visited. If the goal node has been marked visited, then the algorithm is finished and the shortest path has been found.
5. Set the unvisited node marked with the smallest tentative distance as the next "current node" and go back to step 3

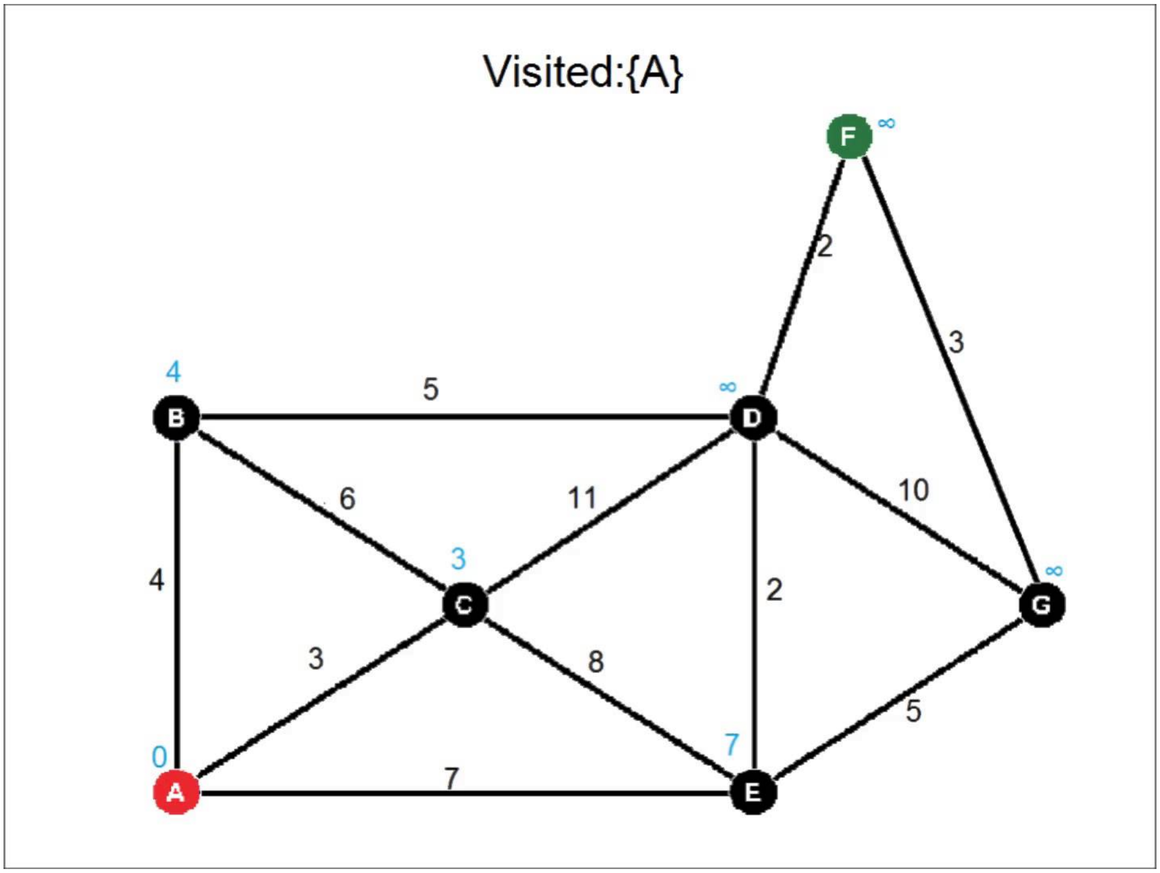


Figure 4: When performing Dijkstra's Algorithm on this example, the shortest path from A to F is given by $A \to B \to D \to F$ with a total cost of 11

Community Detection

Afternoon Goals

- Community Detection Applications
- Measure the quality of a community
  - Modularity
  - Node Similarity
- Divide a graph into communities
  - Divisive Algorithm (Girvan and Newman)
  - Hierarchical Clustering (Agglomerative Algorithm)

Community Quality

The general idea behind trying to quantify the "quality" of a community is that we would like to have the # of edges inside a community be greater than the # of edges between that community and others.

Modularity

A high modularity signifies a "better" community (i.e. a community with high modularity will have dense connections between the nodes of the module, but sparse connections between nodes in a different module).

We calculate this by taking the fraction of edges within a subgraph minus the fraction of edges within the subgraph if all edges were distributed randomly throughout the graph. To be regarded as high modularity, we would expect the edge density to be higher than if they were just randomly assigned throughout the graph.

Randomizing Subgraph

1. Halve each edge (stub) in the subgraph
2. Rewire stubs randomly to other nodes / self node
3. Degree distribution of randomized subgraph will remain the same

$$Q(G,C) = \frac{1}{2m} \sum_{c \in C} \sum_{i,j \in c} A_{ij} - \frac{k_i k_j}{2m}$$

where:

- C: the collection of communities
- m: number of edges in the graph
- A_{ij}: 1 if an edge connects i and j, 0 otherwise
- k_i: degree of node i

Node Similarity

We can say that two nodes are similar if they share many of the same neighbors.

$$n_{ij} = \sum_k A_{ik} A_{kj}$$

- Node similarity is not normalized and fluctuates according to the degree of the nodes
- Usually measure the similarity with **Cosine Similarity** or dissimilarity with **Euclidean Distance**.

Node Dissimilarity: Euclidean Distance

$$d_{ij} = \sum_k (A_{ik} - A_{jk})^2$$

$$normal(d_{ij}) = \frac{d_{ij}}{k_i + k_j}$$

Node Similarity: Cosine Similarity

$$\sigma_{ij} = \frac{n_{ij}}{\sqrt{k_i k_j}}$$

where n_{ij} is the # of shared neighbors and k_i is the degree of node i

How to Divide a Graph

–	Divisive	Agglomerative
Approach	Top-Down	Bottom-Up
Starting Point	Graph	Individual Nodes
Community Formation	Removing Edges	Iteratively merging
Technique	Girvan and Newman	Hierarchical Clustering

Divisive is typically the more popular of these techniques.

Girvan and Newman

This algorithm extends the notion of vertex betweenness to the case of an edge, defining "edge betweenness" of an edge as the number of shortest paths between nodes that run along it.

1. Compute betweenness for all edges
2. Remove edge with largest betweenness (high betweenness = many shortest paths traverse that edge)
3. Recalculate betweenness
4. Calculate modularity if new communities formed
5. Stop if average modularity is maximized (i.e. further iteration would reduce modularity). Otherwise repeat from step 2

Note: The betweenness must be recalculated for each path effected by the removal of an edge. Severe errors will occur if this is not done. For instance, if two communities are connected through multiple edges there is no guarantee that **all** edges will have a high betweenness. All we know is that at least one will have a high betweenness, and thus the other edges must be updated after each iteration.

Agglomerative Algorithm (Hierarchical Clustering)

Merge based on max similarity / minimum distance between elements from each of the two clusters.

- We have to decide the cut-off for hierarchical clustering
- Hierarchy is by construction and not always sensible
- Good for networks that are hierarchical (social / biological)