15-388/688 - Practical Data Science: Graphs and Networks

J. Zico Kolter
Carnegie Mellon University
Fall 2016

Outline

Networks and graph

Representing graphs

Graph algorithms

Graph libraries

Announcements

There have been substantial problems with the autograder for HW2, Problem 1

We are hoping to fix these today, but you may want to hold off on submission until we send an email confirming that the grader is fixed

Participation policy (e.g. negative points for already-answered questions), will not hold for this question, all questions are ok

We don't want to push deadline too much further back, but ***we will allow everyone to use all three late days on assignment (without decreasing late days)***

> ***I.e., new (but hard) deadline is Monday, 10/3***

Outline

Networks and graph

Representing graphs

Graph algorithms

Graph libraries

Networks vs. graphs?

Our terminology (fairly standard, though some use them differently):

Networks are the systems of interrelated objects (in the real world)

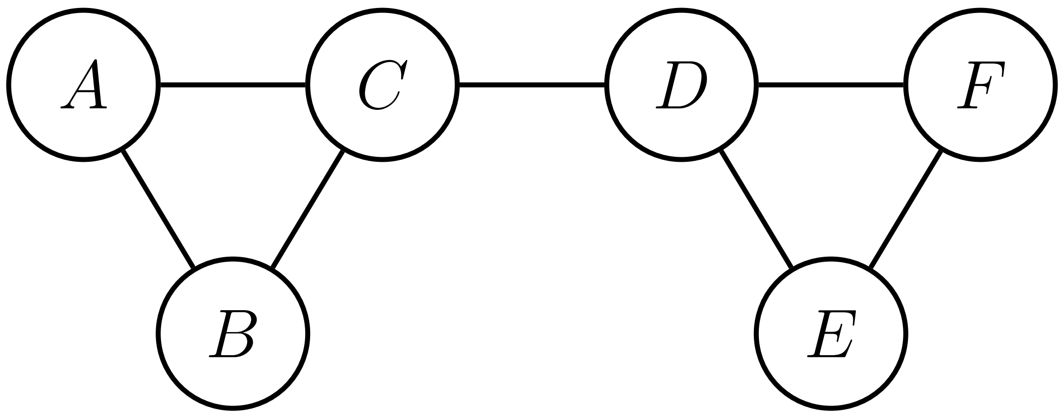
Graphs are the mathematical model for representing networks

This lecture is largely about representations and algorithms for graphs

But of course, in data science we use these algorithms to answer questions about networks

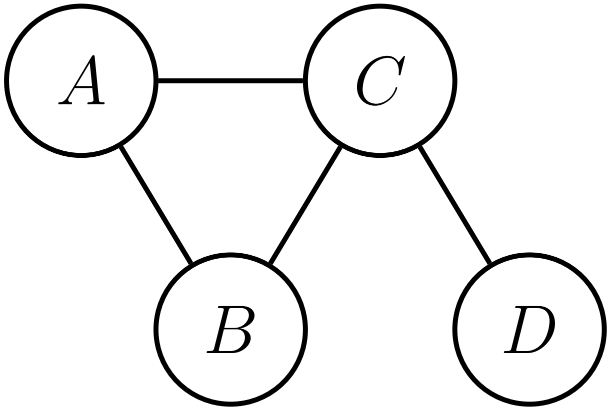
Graphs models

A graph is a collection of vertices (nodes) and edges $G = (V, E)$

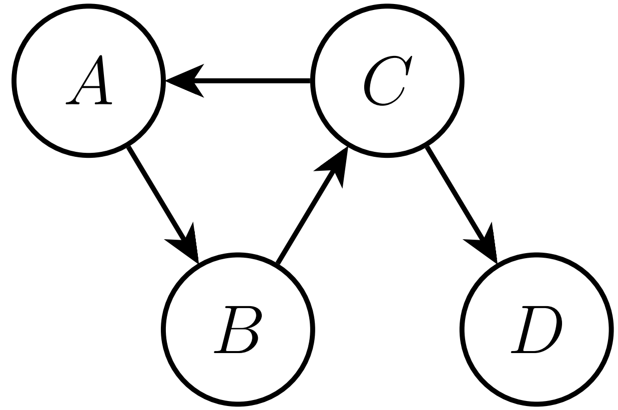


$$V = \{A, B, C, D, E, F\}$$
$$E = \{(A, B), (A, C), (B, C), (C, D), (D, E), (D, F), (E, F)\}$$

Directed vs. undirected graphs

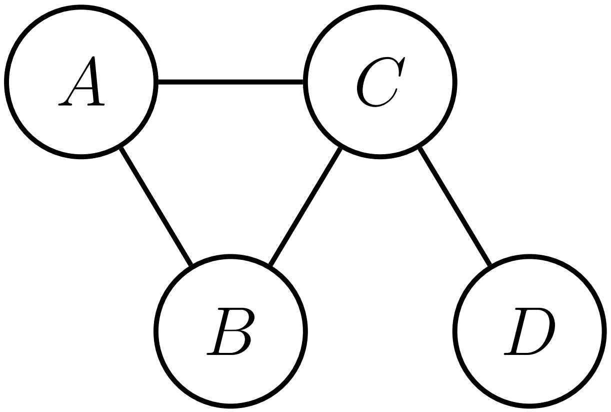


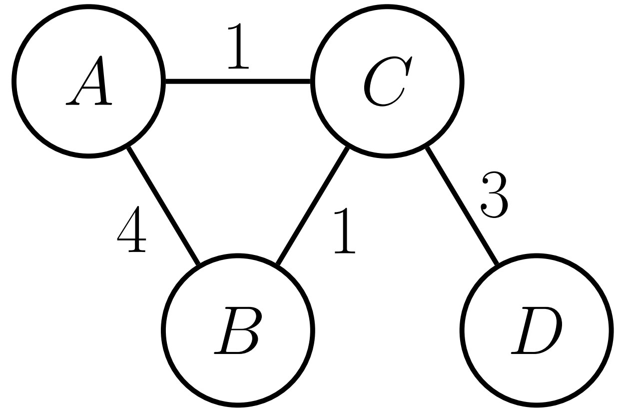
Undirected
E.g. paper co-authorship



Directed
E.g. web links

Weighted vs. unweighted graphs

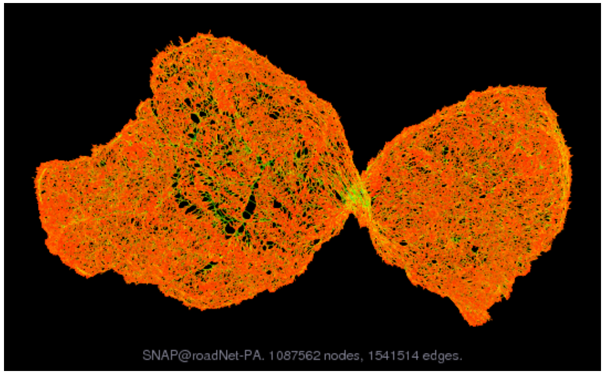




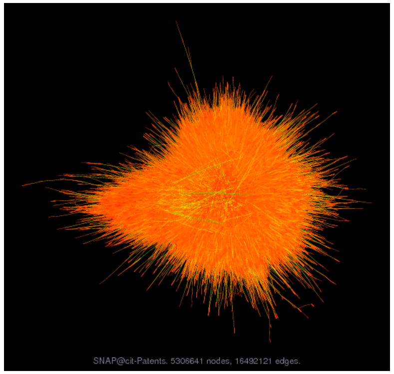
Unweighted
E.g. friends on social network

Weighted
E.g. travel distance between cities

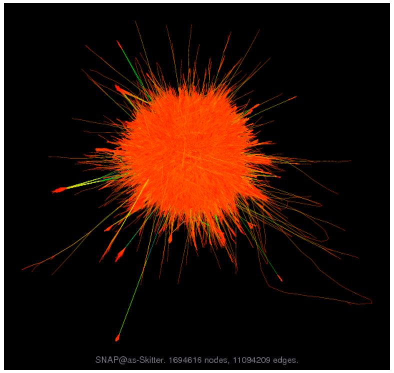
Some example graphs



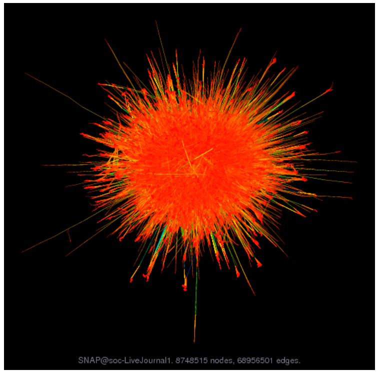
PA road network:
1M nodes, 3M edges



Patent citations:
3.7M nodes, 16.5M edges



Internet topology (in 2005)
1.6M nodes, 11M edges



LiveJournal social network
4.8M nodes, 69M edges

Graphs from http://snap.stanford.edu, visualizations from http://www.cise.ufl.edu/research/sparse/matrices/SNAP/

Outline

Networks and graph

Representing graphs

Graph algorithms

Graph libraries

Representations of graphs

There are a few different ways that graphs can be represented in a program, which one you choose depends on your use case

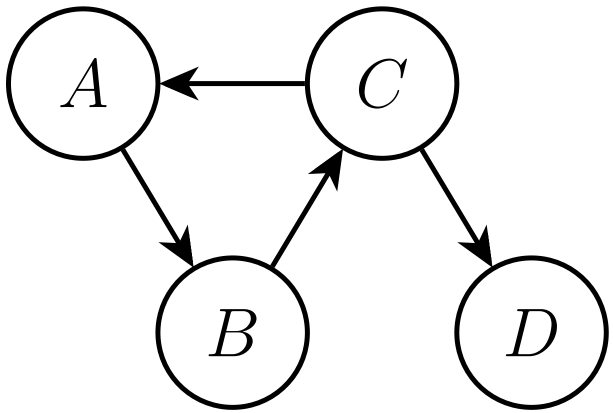
E.g., are you going to be modifying the graph dynamically (adding/removing nodes/edges), just analyzing a static graph, etc?

Three main types we will consider:

1. Adjacency list
2. Adjacency dictionary
3. Adjacency matrix

Adjacency list

For each node, store an array of the nodes that it connects to



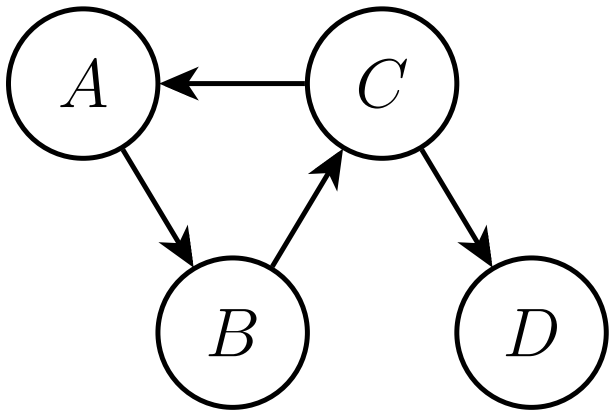
Node	Edges
A	[B]
B	[C]
C	[A,D]
D	[]

Pros: easy to get all outgoing links from a given node, fast to add new edges (without checking for duplicates)

Cons: deleting edges or checking existing of an edge requires scan through given node's full adjacency array

Adjacency dictionary

For each node, store a ***dictionary*** of the nodes that it connects to



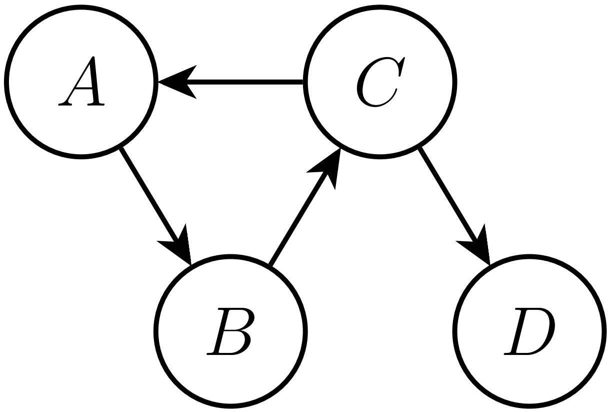
Node (key)	Edges
A	{B:1.0}
B	{C:1.0}
C	{A:1.0,D:1.0}
D	{}

Pros: easy to add/remove/query edges (requires two dictionary lookups, so a $O(1)$ operation)

Cons: overhead of using a dictionary over array

Adjacency matrix

Store the connectivity of the graph as a matrix



$$A = \begin{array}{ccc} \text{(From)} & & \\ \begin{matrix} A & B & C & D \end{matrix} & & \\ \begin{bmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} & \begin{matrix} A \\ B \\ C \\ D \end{matrix} & \text{(To)} \end{array}$$

In virtually all cases, you will want to store this as a sparse matrix

Pros/cons depend on which sparse matrix format you use, but most operations on a static graph will but *much* faster using the right format

Outline

Networks and graph

Representing graphs

Graph algorithms

Graph libraries

Graph algorithms

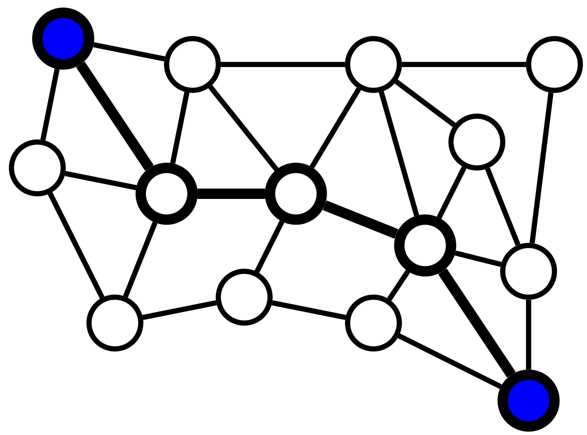
Algorithms for graphs could be (in fact, is) an entire course on its own

We're going to briefly highlight just three algorithms that address different problem classes in graphs

1. Finding shortest paths in a graph – Dijkstra's algorithm
2. Finding important nodes in a graph – PageRank
3. Finding communities in a graph – Girvan-Newman

Shortest path problem

Classical graph problem: find the shortest path between two nodes



Some important distinctions or modifications

- Weighted vs. unweighted, directed vs. undirected, negative weights
- Single-source shortest path (we'll do this one)
- All-pairs shortest path

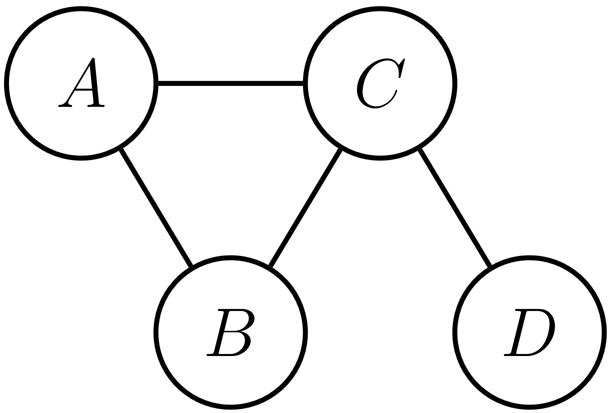
Dijkstra's algorithm

Algorithm for single-source shortest path

Basic idea: dynamic programming algorithm, at each node maintain an *upper bound* on distance to source, iteratively expand node with smallest upper bound (updating bounds of its neighbors)

Given: Graph $G = (V, E)$, Source s
Initialize:
$D[s] \leftarrow 0, \;\; D[i \neq s] \leftarrow \infty$
$Q \leftarrow V$
Repeat until Q empty:
$i \leftarrow$ Remove element from Q with smallest D
For all j such that $(i, j) \in E$:
$D[j] = \min(D[j], D[i] + 1)$

Dijkstra's algorithm example



Initialization: source A

$$D = [0, \infty, \infty, \infty]$$
$$Q = \{A, B, C, D\}$$

Step 1: Pop node A

$$Q = \{B, C, D\}$$
$$D = [0,1,1,\infty]$$

Step 2: Pop node B

$$Q = \{C, D\}$$
$$D = [0,1,1,\infty]$$

Step 3: Pop node C

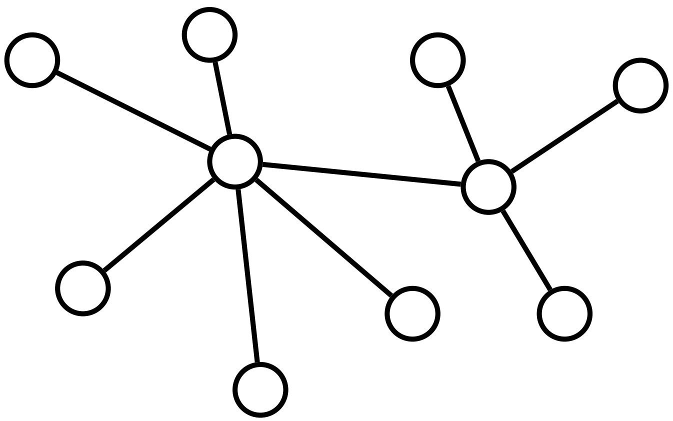
$$Q = \{D\}$$
$$D = [0,1,1,2]$$

Step 4: Pop node D

$$Q = \{\ \}$$
$$D = [0,1,1,2]$$

“Important” nodes

What are the important nodes in the following network?



Unlike shortest path, there is not correct answer here, depends on how you define importance

PageRank algorithm

The algorithm that started Google

Perspective on importance: consider a *random walk* on the graph

- We start at a random node
- We repeatedly jump to a random neighboring node
- If the node has no outgoing edges (in directed graph), jump to a random node
- (Optionally) also jump to a random node with probability d

Node importance is the probability that we will be at a given node when following the above procedure

PageRank algorithm

Given: Graph $G = (V, E)$, restart probability d, iteration count T
Initialize:

$A \leftarrow \mathrm{Adjacency-Matrix}(G)$

$P \leftarrow$ replace zero columns of A with 1, and normalize columns

$\hat{P} \leftarrow (1-d)P + \frac{d}{|V|}11^T$

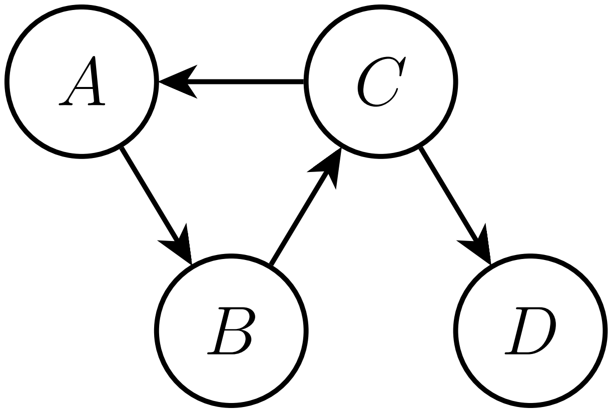
$x \leftarrow \frac{1}{|V|}1$

Repeat T times:

$x \leftarrow \hat{P}x$

For those who have heard these terms, this algorithm is creating a *Markov chain* over the graph, and finding the stationary distribution (largest eigenvector) of this Markov chain

PageRank example

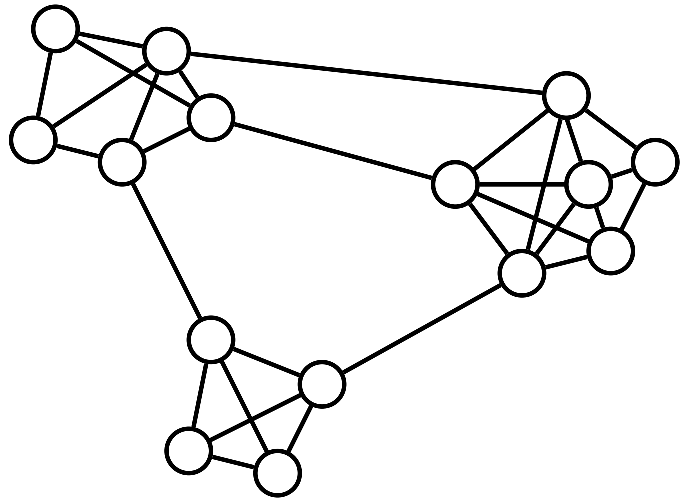


$$A = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \qquad d = 0.9$$

$$P = \begin{bmatrix} 0 & 0 & 0.5 & 0.25 \\ 1 & 0 & 0 & 0.25 \\ 0 & 1 & 0 & 0.25 \\ 0 & 0 & 0.5 & 0.25 \end{bmatrix} \quad \hat{P} = \begin{bmatrix} 0.025 & 0.025 & 0.475 & 0.25 \\ 0.925 & 0.025 & 0.025 & 0.25 \\ 0.025 & 0.925 & 0.025 & 0.25 \\ 0.025 & 0.025 & 0.475 & 0.25 \end{bmatrix} \quad x \to \begin{bmatrix} 0.21 \\ 0.26 \\ 0.31 \\ 0.21 \end{bmatrix}$$

Community detection

Community: subgraphs where nodes are densely connected to each other, but sparsely connected to other nodes



A “soft” version of a clique (a fully connected subgraph)

A fundamental concept in e.g. social networks

Girvan-Newman Algorithm

Published in 2002 (Girvan and Newman, 2002), one of the first methods of "modern" community detection

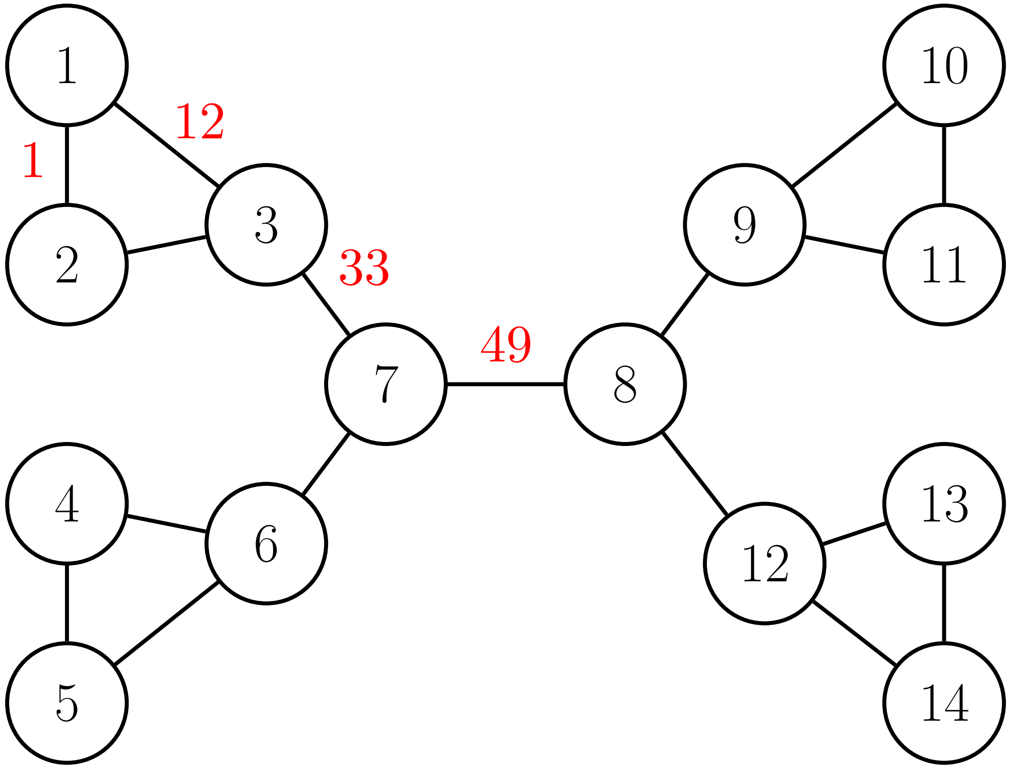
Basic idea: Recursively partition the network by removing edges, groups that are last to be partitioned are "communitites"

1. Compute "betweenness" of edges in the network = number of shortest paths that pass through each edge
2. Remove edge(s) with highest betweenness, if this breaks the graph into subgraphs, recursively partition each one

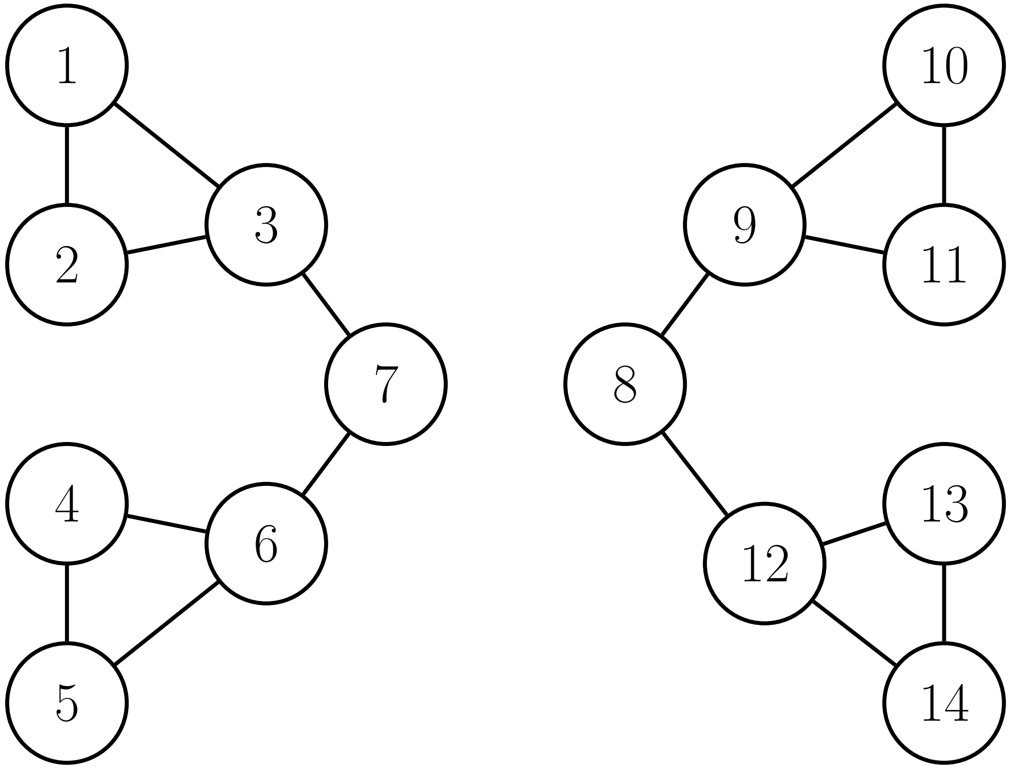
Challenge is efficiently computing betweenness as we partition graph (we will not cover this)

Result is a hierarchical partitioning of the graph

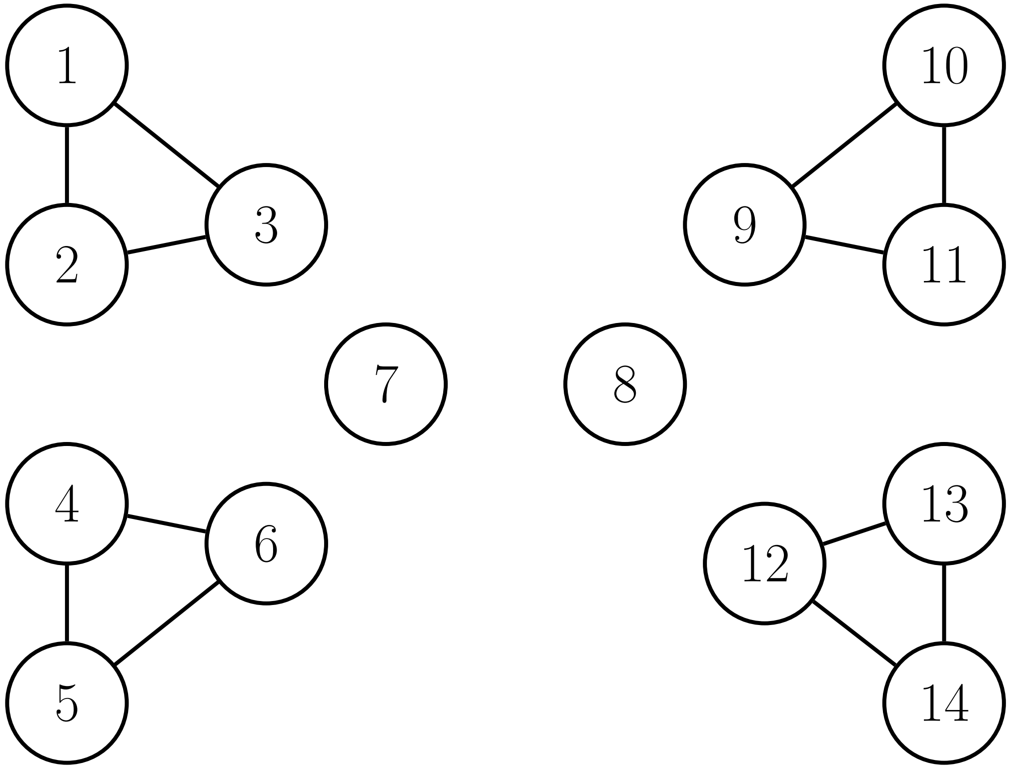
Algorithmic illustration



Algorithmic illustration



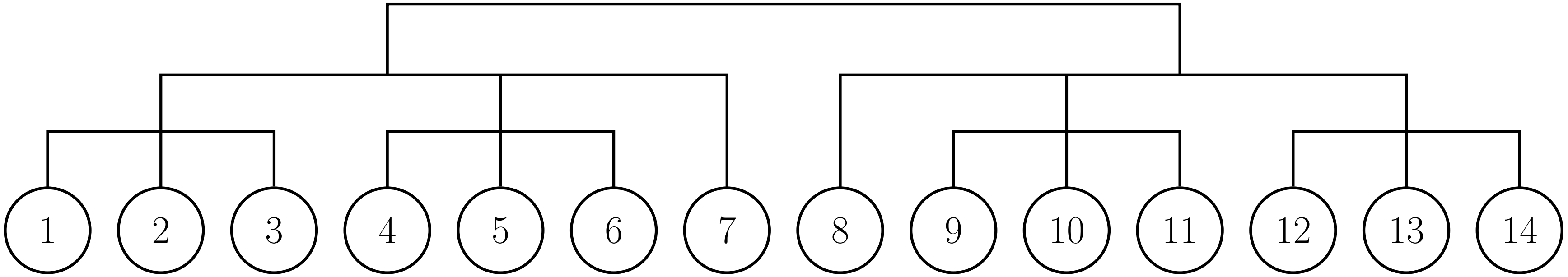
Algorithmic illustration



Resulting hierarchy (dendrogram)

Communities can be extracted by looking at the grouping at different levels of the tree

May want to threshold on things like community size, etc



Outline

Networks and graph

Representing graphs

Graph algorithms

Graph libraries

NetworkX

NetworkX: Python library for dealing with (medium-sized) graphs

https://networkx.github.io/

Simple Python interface for constructing graph, querying information about the graph, and running a large suite of algorithms

Not suitable for very large graphs (all native Python, using adjacency dictionary representation)

Creating graphs

Create an undirected or directed graph

```
import networkx as nx

G = nx.Graph()   # undirected graph
G = nx.DiGraph() # directed graph
```

Add and remove nodes/edges

```
# add and remove edges
G.add_edges_from([("A","B"), ("B","C"), ("C","A"), ("C","D")])
G.remove_edge("A","B")
G.add_edge("A","B")
G.remove_edges_from([("A","B"), ("B","C")])
G.add_edges_from([("A","B"), ("B","C")])
# also add_node(), remove_node(), add_nodes_form(), remove_nodes_from()
```

Nodes/edges and properties

NetworkX uses adjacency dictionary format internally

```
print G["C"]
# {'A': {}, 'D': {}}
```

Iterate over nodes and edges

```
for i in G.nodes():     # loop over nodes
    print i
for i,j in G.edges():   # loop over edges
    print i,j
```

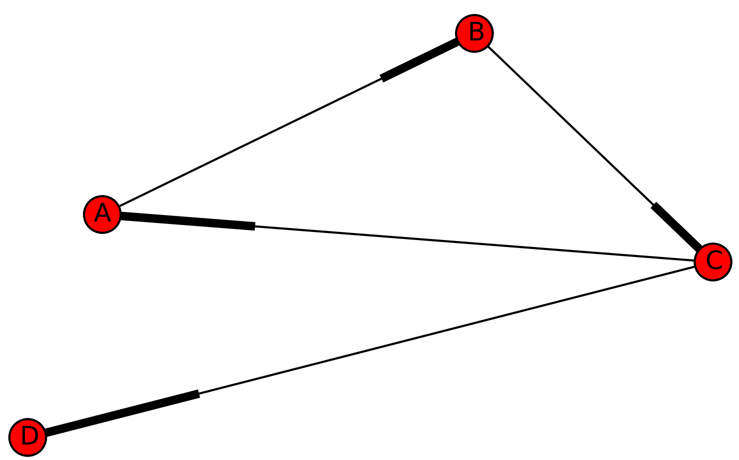
Get and set node/edge properties

```
G.node["A"]["node_property"] = "node_value"
G.edge["A"]["B"]["edge_property"] = "edge_value"
G.nodes(data=True) # iterator over nodes returning properties
G.edges(data=True) # iterator over edges returning properties
```

Drawing and node properties

Draw a graph using matplotlib (not the best visualization)

```
import matplotlib.pyplot as plt
%matplotlib inline
nx.draw(G,with_labels=True)
plt.savefig("mpl_graph.pdf")
```



Algorithms

Almost all the (medium scale) algorithms you could want

```
nx.shortest_path_length(G,source="A") # iterater over path lengths

nx.pagerank(G,alpha=0.9) # dictionary of node ranks

# NOTE: this requires Networkx 2.0dev
# pip install --upgrade git+git://github.com/networkx/networkx.git
nx.girvan_newman(G) # iterator over partitions at
                      different hierarchy levels
```