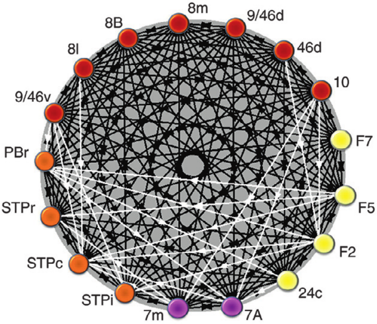
CS 6824: Components, Cliques, and Cores

T. M. Murali

February 15 and 20, 2018



Summary of Course Thus Far

- History of neuroscience
- Graphs (Definitions, basic concepts, Euler tours)
- Brain graphs (types of nodes and edges, experimental methods, Chapter 2)
- Brain connectivity matrices and node degrees (Chapters 3 and 4)
- Shortest paths (Chapter 7.1 and 7.2)
- Clustering coefficient and small world networks (Chapter 8.1 and 8.2)

Plan till Spring Break

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Are there intermediate notions of graph density?

- Subgraphs that represent backbones of network topology (components, shortest paths, spanning trees, cores, Chapter 6.1, 6.2, 7.1, February 15 and 20)
- Modularity (Chapter 9, February 22, 27, March 1)

Student Presentations

- I have provided a list of topics (roughly corresponding to textbook sections) for student presentations on the course website.
- Each group should give me its top three choices by 5pm on Tuesday, February 20.
- I will assign one topic to each group by February 22.
- I will also add the topics to the course schedule.

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- Each group meets me for 60–90 minutes about two weeks before practice presentation.
  - I will announce office hours and a schedule for these meetings.
  - Goal is to discuss details of presentation.
  - Come prepared: read your section, find relevant papers, have a talk outline, ask me quesitons.
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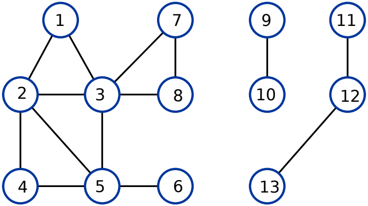
- Projects to be announced before spring break.

Plan after Spring Break

- Two invited presentations by Heidi Theussen from Smith Career Center (March 15 and 17)
- Practice presentations (March 20 to April 5, with one practice presentation held outside class hours)
- Presentations (April 10 to May 1)

Paths and Connectivity



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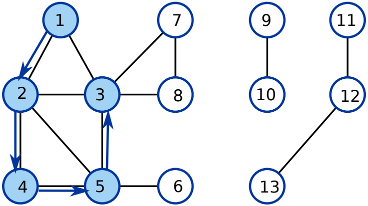

- A *v_1-v_k path* in an undirected graph $G = (V, E)$ is a sequence P of nodes $v_1, v_2, \ldots, v_{k-1}, v_k \in V$ such that every consecutive pair of nodes $v_i, v_{i+1}, 1 \leq i < k$ is connected by an edge in E.

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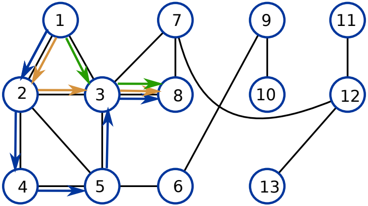

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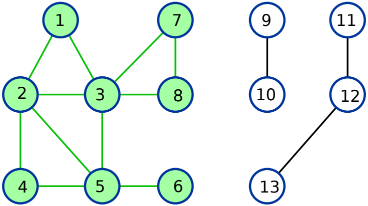

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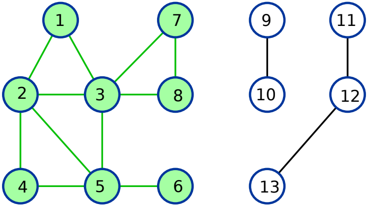

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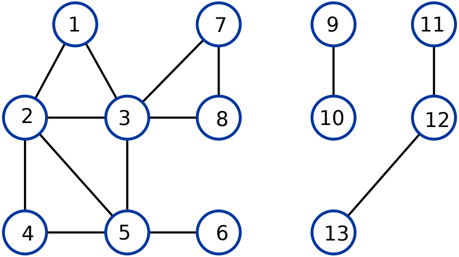
Breadth-First Search (BFS)



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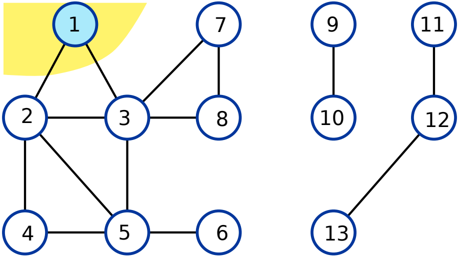

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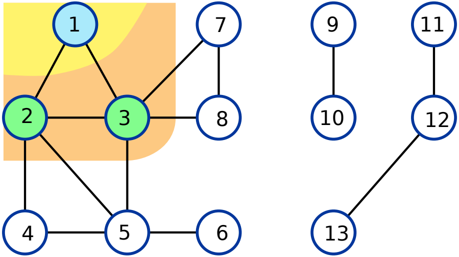

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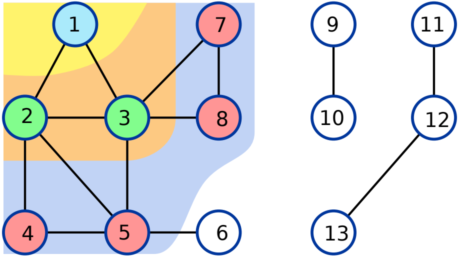

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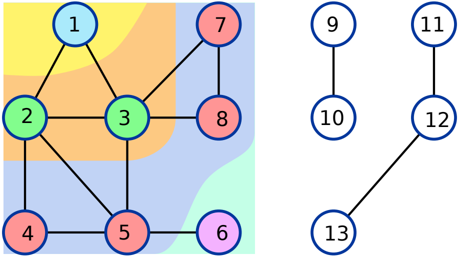

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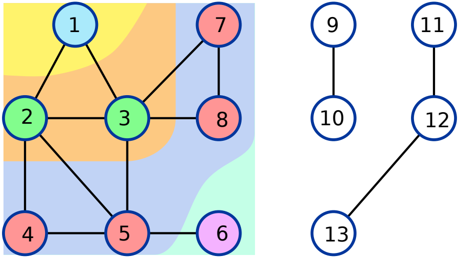
Properties of BFS



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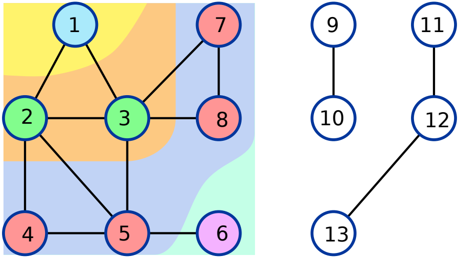

- For each $j \geq 1$, layer L_j consists of all nodes exactly at distance j from S.
- There is a path from s to t if and only if t is a member of some layer.

Implementing BFS

- Maintain an array Discovered and set Discovered$[v]$ = *true* as soon as the algorithm sees v.

```
BFS(s):
  Set Discovered[s] = true and Discovered[v] = false for all other v
  Initialize L[0] to consist of the single element s
  Set the layer counter i = 0
  Set the current BFS tree T = Ø
  While L[i] is not empty
    Initialize an empty list L[i + 1]
    For each node u ∈ L[i]
      Consider each edge (u, v) incident to u
      If Discovered[v] = false then
        Set Discovered[v] = true
        Add edge (u, v) to the tree T
        Add v to the list L[i + 1]
      Endif
    Endfor
    Increment the layer counter i by one
  Endwhile
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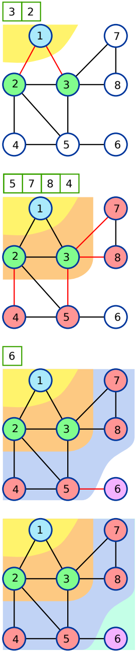

Using a Queue in BFS

- Instead of storing each layer in a different list, maintain all the layers in a single queue L.
- We can guarantee that all nodes in layer i will be put in the queue after every node in layer $i-1$ and before every node in layer $i+1$.

```
BFS(s):
   Set Discovered[s] = true
   Set Discovered[v] = false, for all other nodes v
   Initialize L to consist of the single element s
   While L is not empty
       Pop the node u at the head of L
       Consider each edge (u, v) incident on u
       If Discovered[v] = false then
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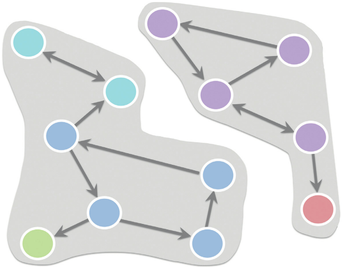
- Time used by `for` loop for a node u: $O(d(u))$ time.
- Total time for all `for` loops: $\sum_{u \in G} O(d(u)) = O(m)$ time.
- Total time is $O(n + m)$.

Connected Components in Directed Graphs



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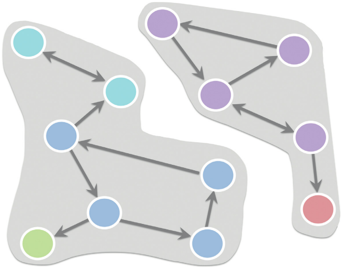

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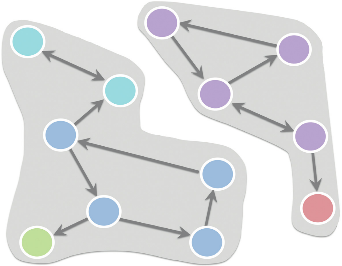

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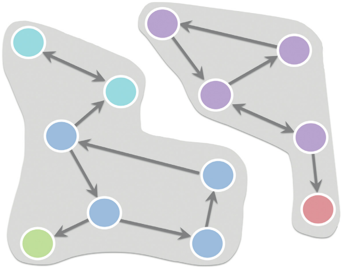
- We can compute all weakly connected components in linear time.

Connected Components in Directed Graphs



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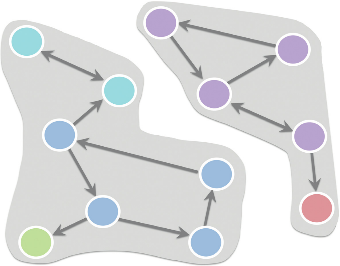

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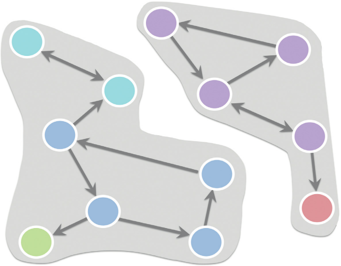

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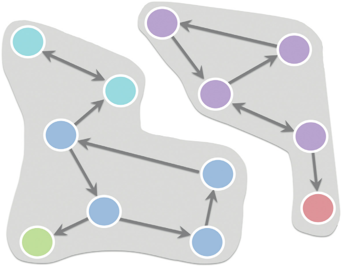

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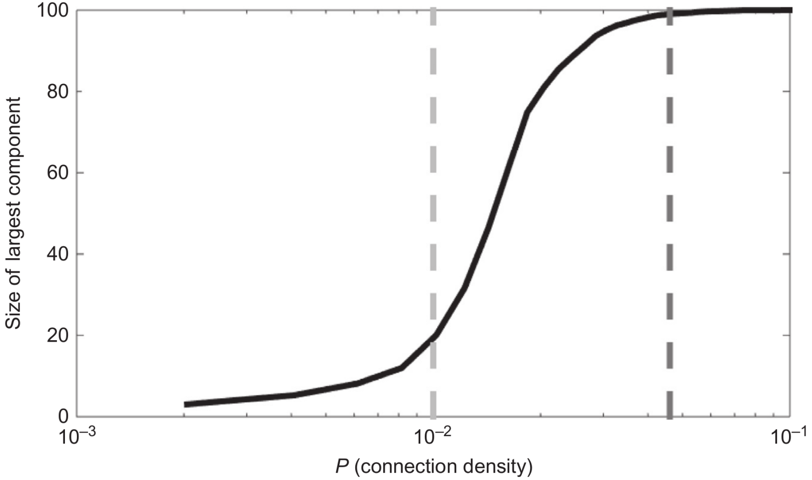
  - H is *maximal*, i.e., for every node $x \in V - V'$, there is at least one node $y \in V'$ such that there is no path in G from x to y or from y to x.
- We can compute all strongly connected components in linear time using DFS with some tricks.

Largest Component in Brain Graphs



- Phase transition for appearance of large component in E-R graphs.

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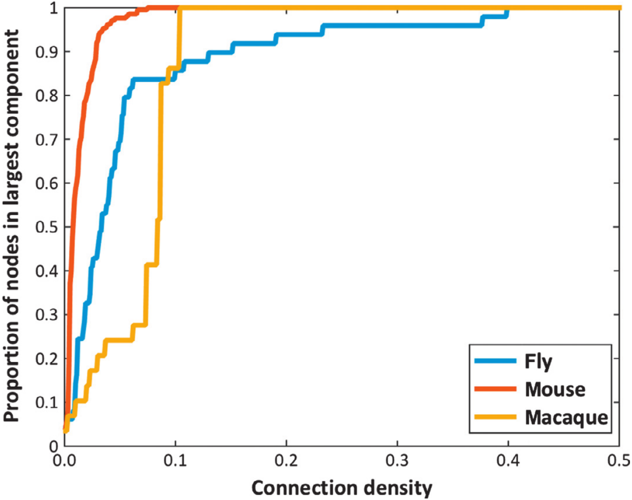

- Add edges in decreasing order of weight.
- Plot the size of the largest weakly connected component.

Shortest Paths Problem

- $G(V, E)$ is a directed graph. Each edge e has a length $l(e) \geq 0$.
- V has n nodes and E has m edges.
- *Length of a path* P is the sum of the lengths of the edges in P.
- Goal is to determine the shortest path from a specified start node s to each node in V.
- Aside: If G is undirected, convert to a directed graph by replacing each edge in G by two directed edges.

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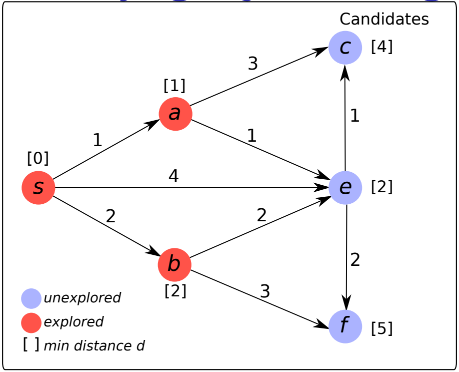
SHORTEST PATHS

Given a directed graph $G(V, E)$, a function $l : E \rightarrow \mathbb{R}^+$, and a node $s \in V$,

compute a set $\{P(u), u \in V\}$, where $P(u)$ is the shortest path in G from s to u.

Idea Underlying Dijkstra's Algorithm



- Maintain a set S of explored nodes.
  - For each node $u \in S$, compute a value $d(u)$, which (we will prove) is the length of the shortest path from s to u.
  - For each node $x \notin S$, maintain a value $d'(x)$, which is the length of the shortest path from s to x using only the nodes in S (and x, of course). $d'(x)$ is an upper bound on the $d(x)$

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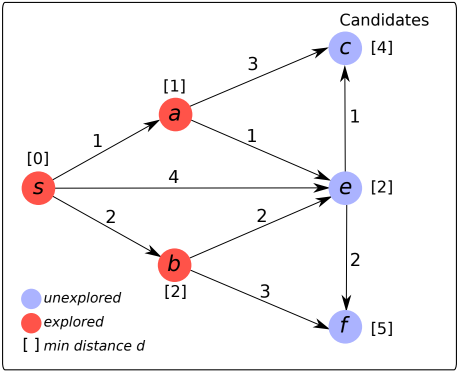
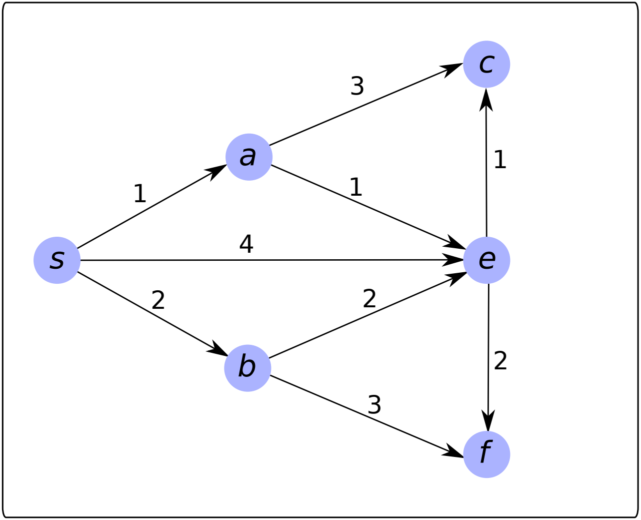


- Maintain a set S of explored nodes.
- "Greedily" add a node v to S that has the smallest value of $d'(v)$ (is closest to s using only nodes in S).
- Prove that at the moment we add v to S, $d(v) = d'(v)$.

Example of Dijkstra's Algorithm



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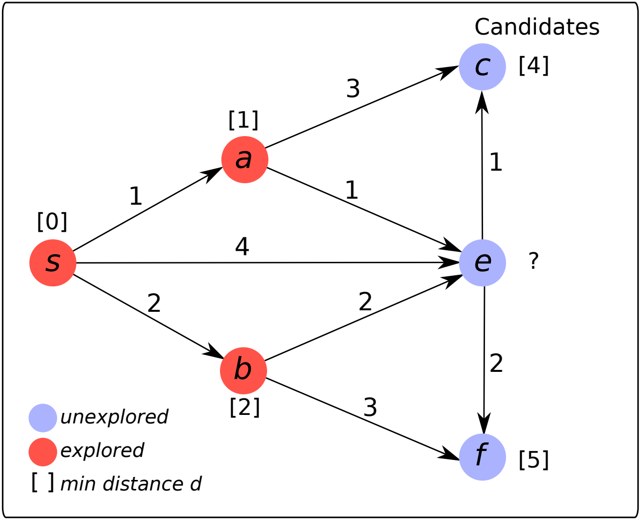

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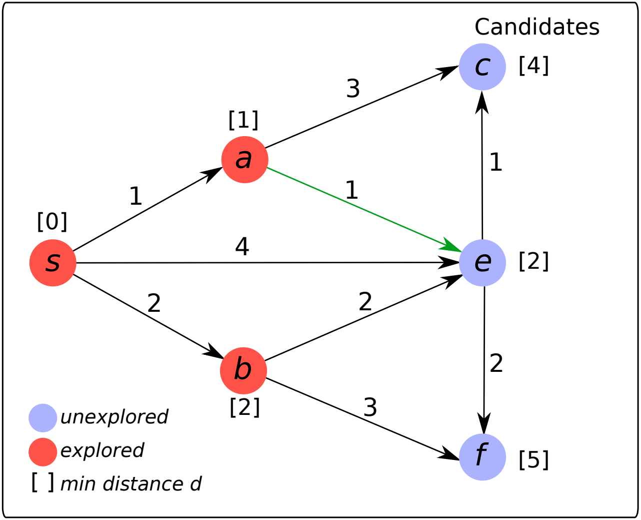

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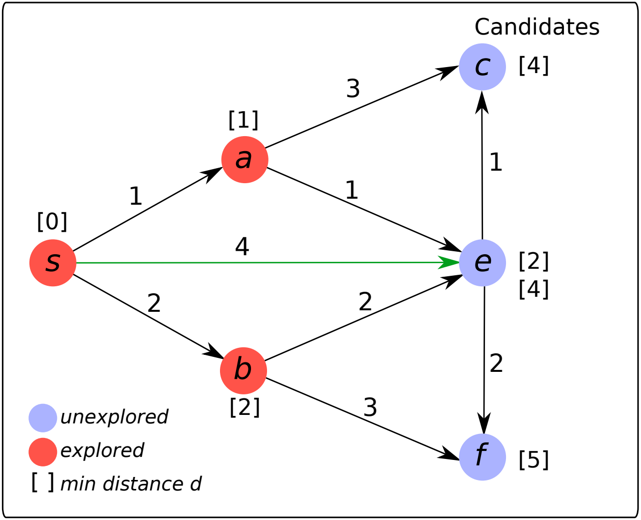

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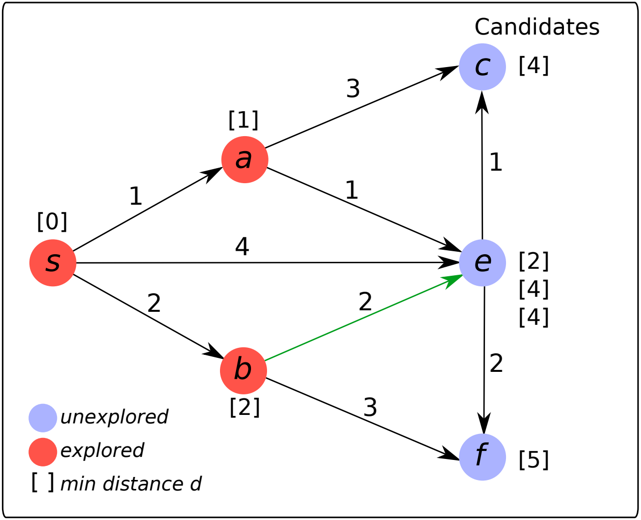

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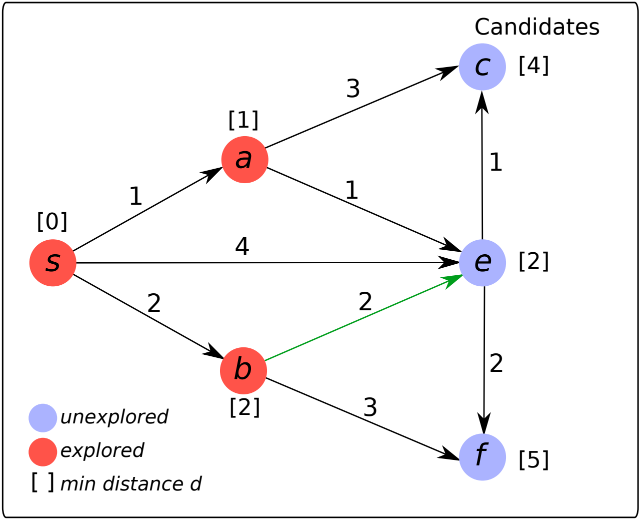

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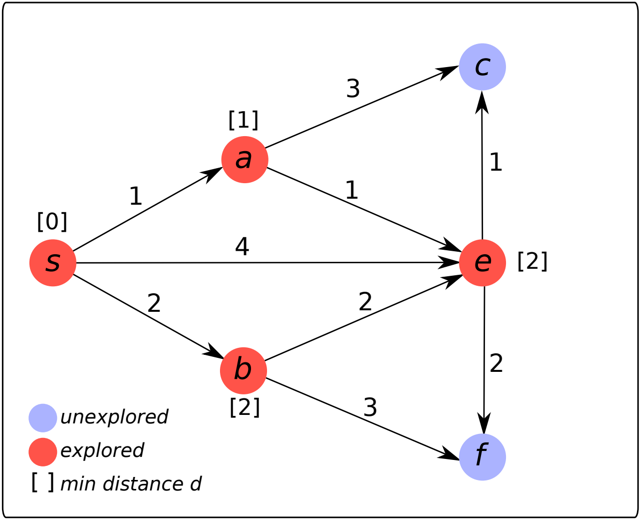

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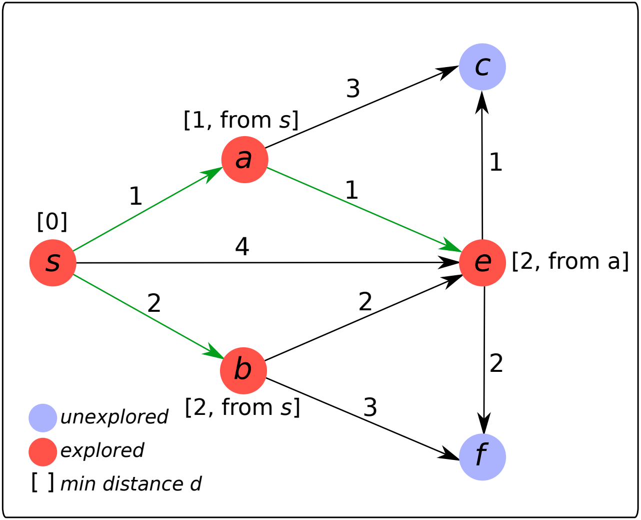

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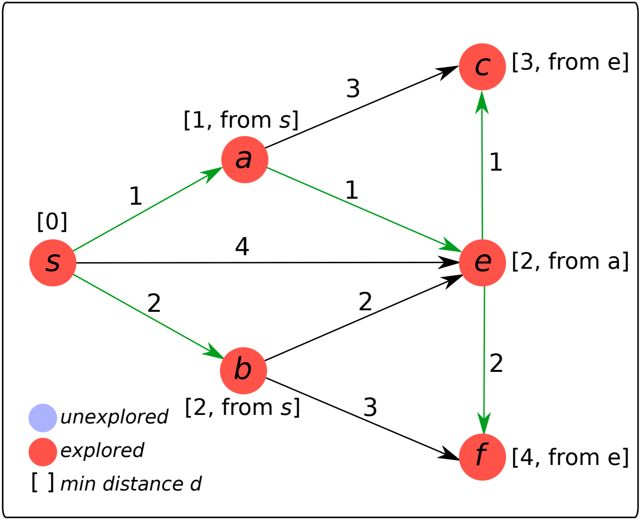

Dijkstra's Algorithm

DIJKSTRA'S ALGORITHM(G, l, s)

1: $S = \{s\}$ and $d(s) = 0$
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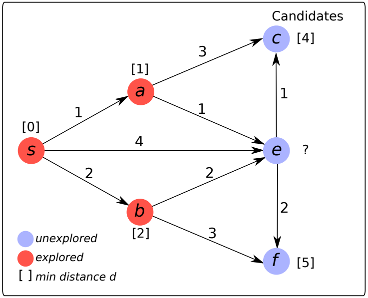

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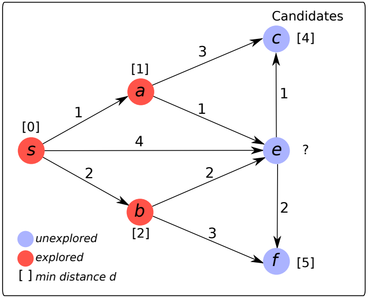

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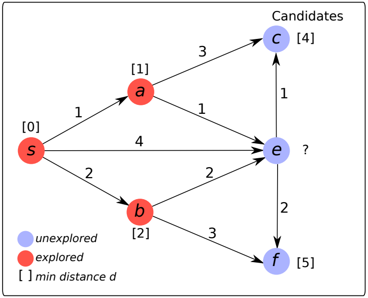

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  - The algorithm is examining a particular (unexplored) node x in $V - S$.

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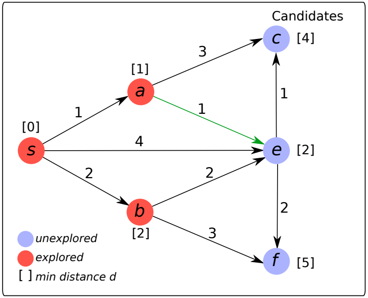

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Dijkstra's Algorithm

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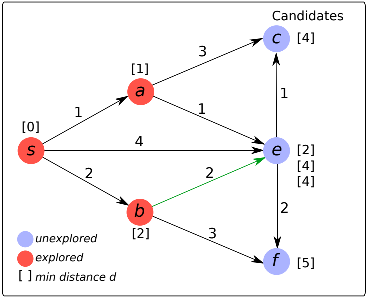

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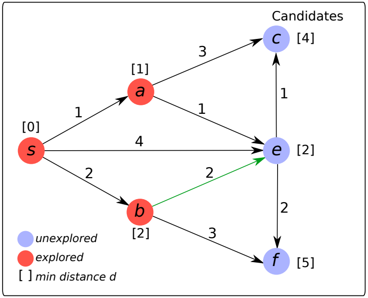

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  - We store the smallest of these values in $d'(x)$.

Dijkstra's Algorithm

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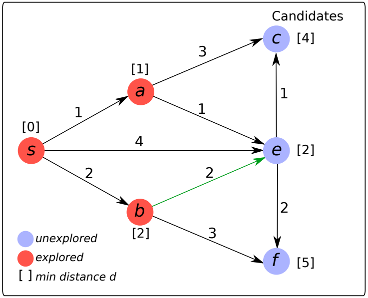

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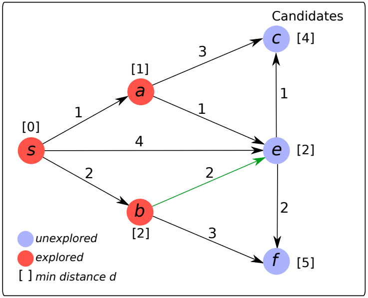

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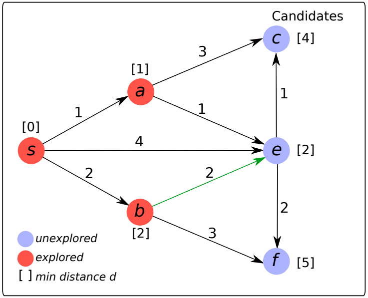

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  - Examine the d' values for these nodes.

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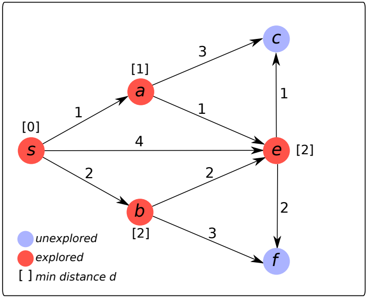

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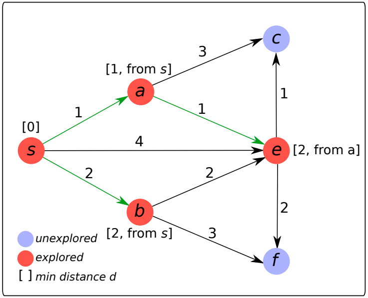

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  - Run over all (unexplored) nodes x in $V - S$.
  - Examine the d' values for these nodes.
  - Return the *argument* (i.e., the node) that has the smallest value of $d'(x)$.
- To compute the shortest paths: when adding a node v to S, store the predecessor u that minimises $d'(v)$.

Proof of Correctness

- Let $P(u)$ be the path computed by the algorithm for a node u.
- Claim: $P(u)$ is the shortest path from s to u.
- Prove by induction on the size of S, i.e., follow the algorithm.

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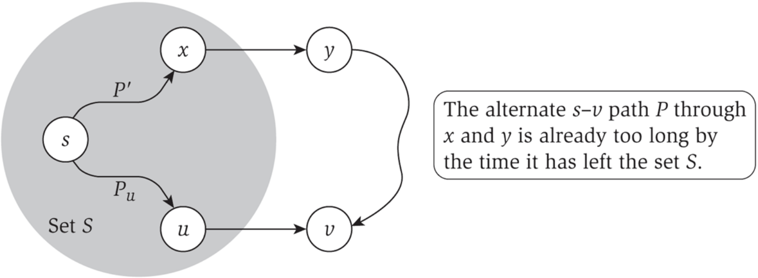

A Faster implementation of Dijkstra's Algorithm

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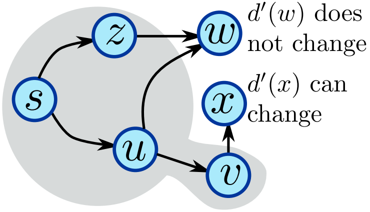

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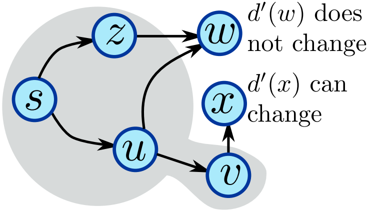

- Observation: If we add v to S, $d'(x)$ changes only if (v, x) is an edge in G.

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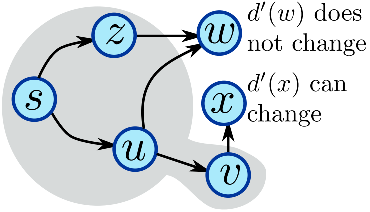

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- Idea: For each node $x \in V - S$, store the current value of $d'(x)$. Upon adding a node v to S, update $d'()$ only for neighbours of v.

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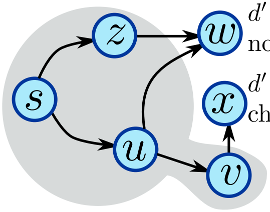

$d'(w)$ does not change

$d'(x)$ can change

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- Idea: For each node $x \in V - S$, store the current value of $d'(x)$. Upon adding a node v to S, update $d'()$ only for neighbours of v.
- How do we efficiently compute $v = \arg\min_{x \in V-S} d'(x)$?

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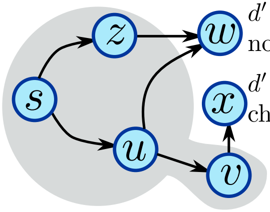

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- How do we efficiently compute $v = \arg\min_{x \in V-S} d'(x)$?
- Use a priority queue!

Faster Dijkstra's Algorithm

DIJKSTRA'S ALGORITHM(G, l, s)

1: INSERT$(Q, s, 0)$.
2: **while** $S \neq V$ **do**
3: $(v, d'(v)) =$ EXTRACTMIN(Q)
4: Add v to S and set $d(v) = d'(v)$
5: **for** every node $x \in V - S$ such that (v, x) is an edge in G **do**
6: **if** $d(v) + l(v, x) < d'(x)$ **then**
7: $d'(x) = d(v) + l(v, x)$
8: CHANGEKEY$(Q, x, d'(x))$

- For each node $x \in V - S$, store the pair $(x, d'(x))$ in a priority queue Q with $d'(x)$ as the key.
- Determine the next node v to add to S using EXTRACTMIN (line 3).
- After adding v to S, for each node $x \in V - S$ such that there is an edge from v to x, check if $d'(x)$ should be updated, i.e., if there is a shortest path from s to x via v (lines 5–8).
- In line 8, if x is not in Q, simply insert it.

Running Time of Faster Dijkstra's Algorithm

DIJKSTRA'S ALGORITHM(G, l, s)

```
INSERT(Q, s, 0).
while S ≠ V do
    (v, d'(v)) = EXTRACTMIN(Q)
    Add v to S and set d(v) = d'(v)
    for every node x ∈ V − S such that (v, x) is an edge in G do
        if d(v) + l_(v,x) < d'(x) then
            d'(x) = d(v) + l_(v,x)
            CHANGEKEY(Q, x, d'(x))
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- How many invocations of EXTRACTMIN?

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- How many invocations of EXTRACTMIN? $n - 1$.

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- How many invocations of EXTRACTMIN? $n - 1$.
- For every node v, what is the running time of step 5?

Running Time of Faster Dijkstra's Algorithm

Dijkstra's Algorithm(G, l, s)

1: Insert$(Q, s, 0)$.
2: **while** $S \neq V$ **do**
3: $(v, d'(v)) =$ ExtractMin(Q)
4: Add v to S and set $d(v) = d'(v)$
5: **for** every node $x \in V - S$ such that (v, x) is an edge in G **do**
6: **if** $d(v) + l_{(v,x)} < d'(x)$ **then**
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- How many invocations of ExtractMin? $n - 1$.
- For every node v, what is the running time of step 5? $O(d_{\text{out}}(v))$, the number of *outgoing* neighbours of v.

Running Time of Faster Dijkstra's Algorithm

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- How many invocations of EXTRACTMIN? $n - 1$.
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- How many invocations of EXTRACTMIN? $n - 1$.
- For every node v, what is the running time of step 5? $O(d_{\text{out}}(v))$, the number of *outgoing* neighbours of v.
- What is the total running time of step 5? $\sum_{v \in V} O(d_{\text{out}}(v)) = O(m)$.

Running Time of Faster Dijkstra's Algorithm

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5:     for every node x ∈ V − S such that (v, x) is an edge in G do
6:         if d(v) + l_(v,x) < d'(x) then
7:             d'(x) = d(v) + l_(v,x)
8:             ChangeKey(Q, x, d'(x))
```

- How many invocations of EXTRACTMIN? $n - 1$.
- For every node v, what is the running time of step 5? $O(d_{\text{out}}(v))$, the number of *outgoing* neighbours of v.
- What is the total running time of step 5? $\sum_{v \in V} O(d_{\text{out}}(v)) = O(m)$.
- How many times does the algorithm invoke CHANGEKEY?

Running Time of Faster Dijkstra's Algorithm

DIJKSTRA'S ALGORITHM(G, l, s)

```
1: INSERT(Q, s, 0).
2: while S ≠ V do
3:     (v, d'(v)) = EXTRACTMIN(Q)
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5:     for every node x ∈ V − S such that (v, x) is an edge in G do
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- How many times does the algorithm invoke CHANGEKEY? $\leq m$.
- What is total running time of the algorithm? $O(m \log n)$.

Graph Measures Based on Shortest Paths

- *Characteristic path length* $l(G)$ is the average shortest path length between all pairs of nodes in G. $\delta(u, v)$ = shortest path length from u to v.

$$l(G) = \frac{1}{n(n-1)} \sum_{u,v \in V, u \neq v} \delta(u, v)$$

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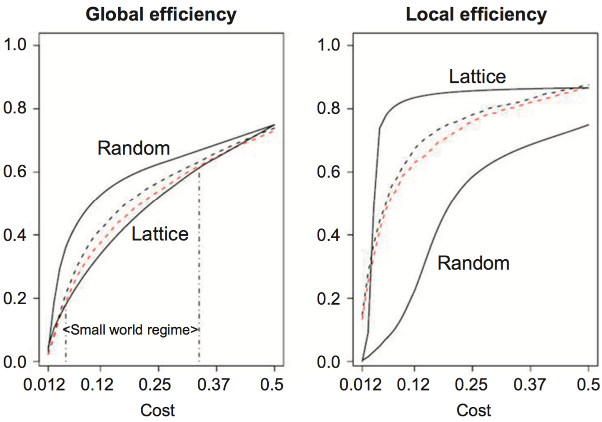
- *Global efficiency* $e_{\mathrm{glob}}(G)$ is the average of the reciprocal of the shortest path length between all pairs of nodes in G.

$$e_{\mathrm{glob}}(G) = \frac{1}{n(n-1)} \sum_{u,v \in V, u \neq v} \frac{1}{\delta(u, v)}$$

- *Local efficiency* $e_{\mathrm{loc}}(v)$ of a node v is the average of the reciprocal of the shortest path length between all pairs of neighbours of v in G.

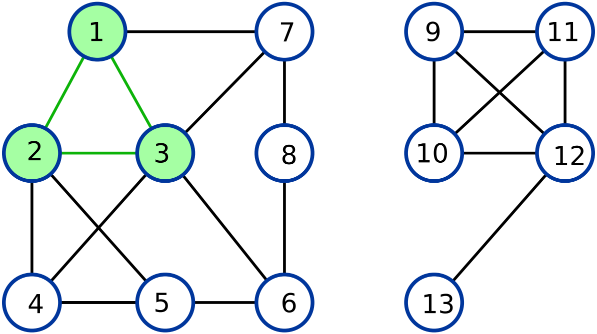
$$e_{\mathrm{loc}}(v) = \frac{1}{d(v)(d(v)-1)} \sum_{\substack{u,v \in N(v) \\ u \neq v}} \frac{1}{\delta(u, v)}$$

Efficiency in Brain Networks



- Functional connectivity networks from fMRI data in young (black) and old (orange) human volunteers.
- *x*-axis is fraction of possible edges as threshold on edge weight varies.
- *y*-axis is global (left) and local (right) efficiency.
- Small world networks are both locally and globally efficient.

Defining Modules



- How do we define a module in an undirected graph?
- In an undirected graph $G = (V, E)$, a subset of nodes $C \subseteq V$ is a *clique* or *complete subgraph* if for every pair of nodes $u, v \in C$, (u, v) is an edge in E.

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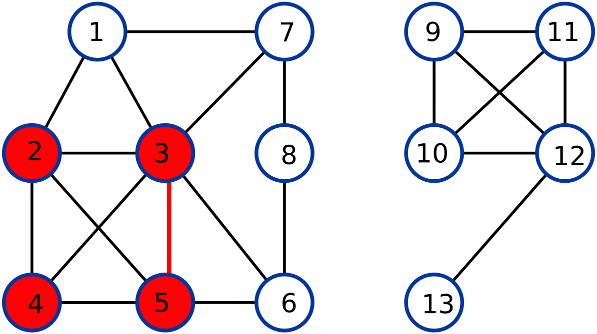

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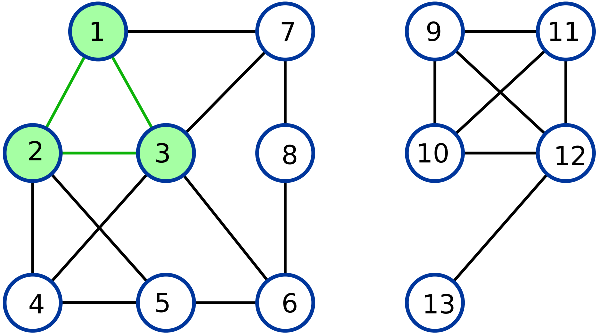

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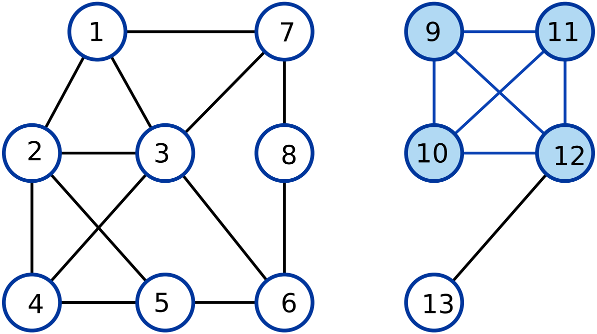

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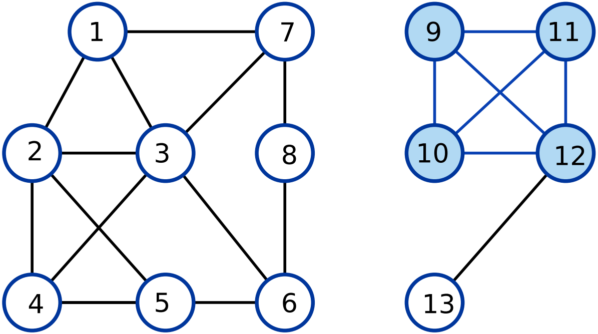
  - A clique C is *maximum* if there is no clique C' in G with more nodes than C.

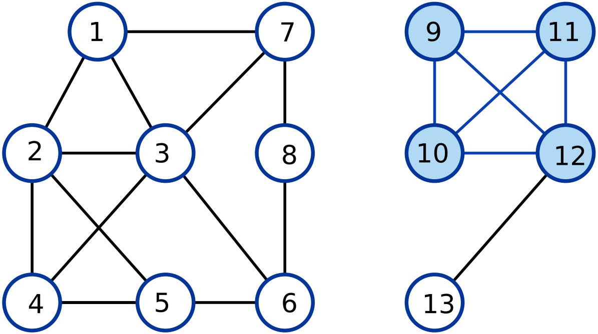
Computing a Maximum Clique



MAXIMUM CLIQUE

Given an undirected, unweighted graph $G(V, E)$, compute the largest clique in G.

Computing a Maximum Clique

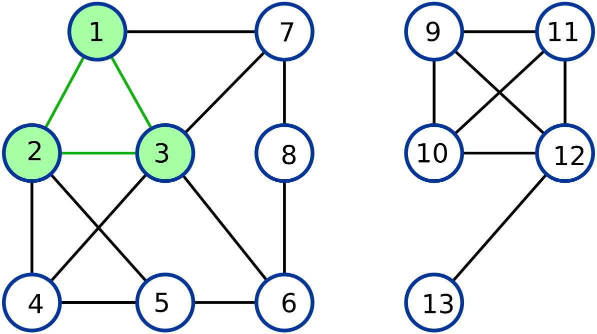


Maximum Clique

Given an undirected, unweighted graph $G(V, E)$, compute the largest clique in G.

- Computing a maximum clique is NP-hard.
- Any algorithm that can provably compute the maximum clique is likely to have a running time that is exponential in the size of the graph.

Computing a Maximal Clique



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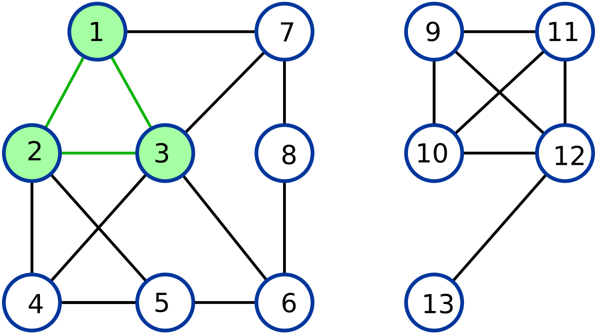

MAXIMAL CLIQUE

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1. Select an arbitrary node v and add it to S (the clique we will output).
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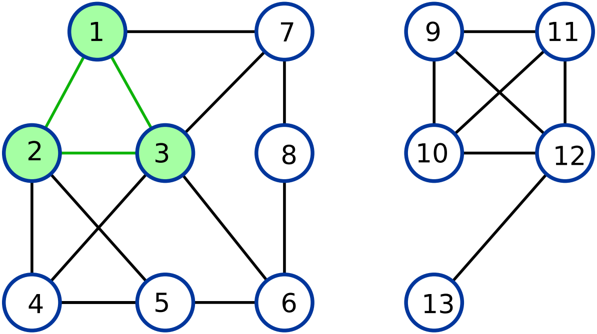
3. Repeat the previous step until no such node u is found.

Running Time to Compute a Maximal Clique



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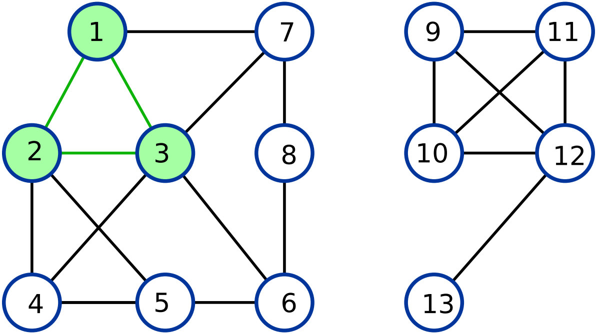

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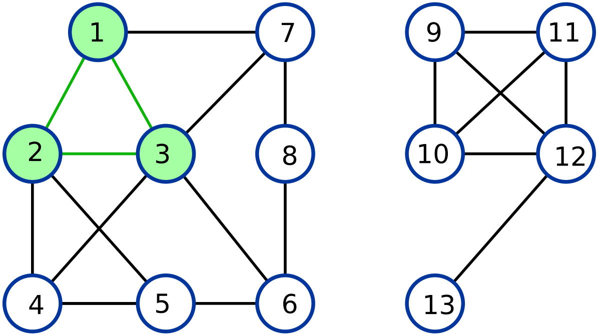

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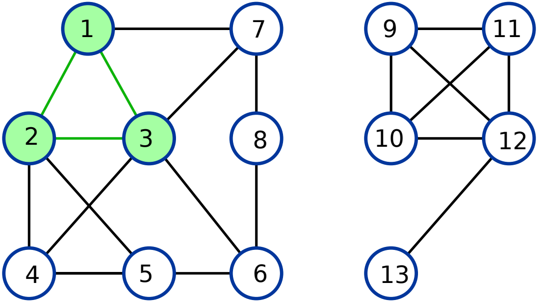
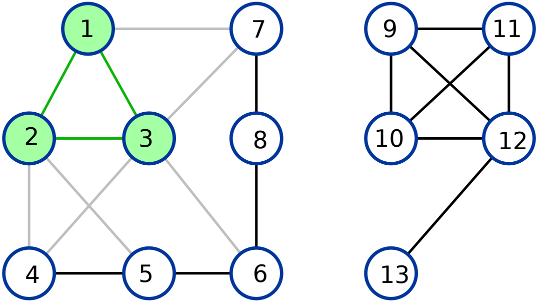
Clique Decomposition



- What do we do after computing a maximal clique?

Clique Decomposition



- What do we do after computing a maximal clique?
- Delete nodes in that clique from the graph and repeat.

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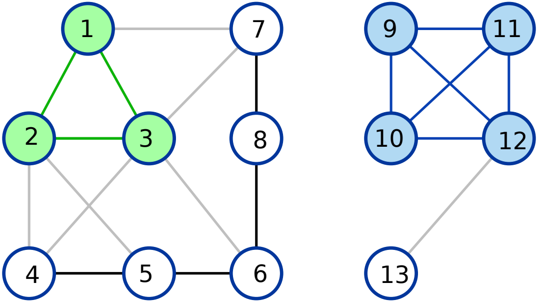

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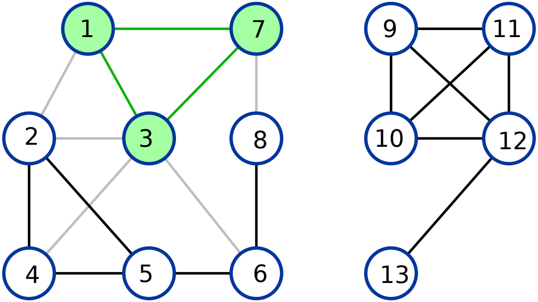
- The resulting set of cliques forms a *clique decomposition* of G.

Clique Decomposition



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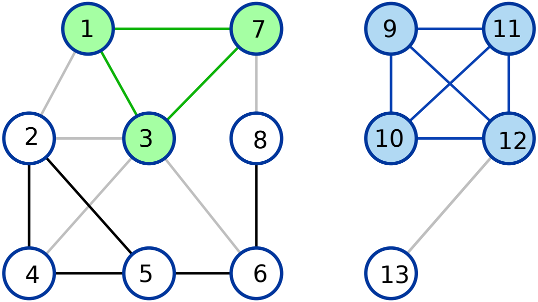

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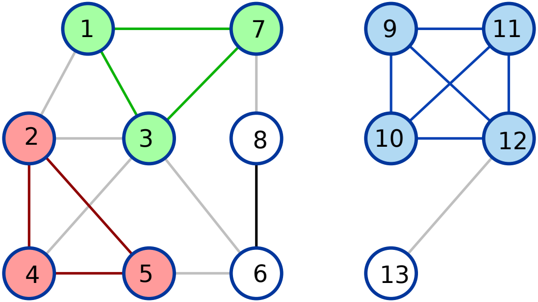

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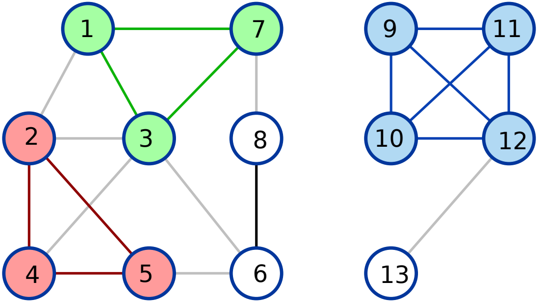

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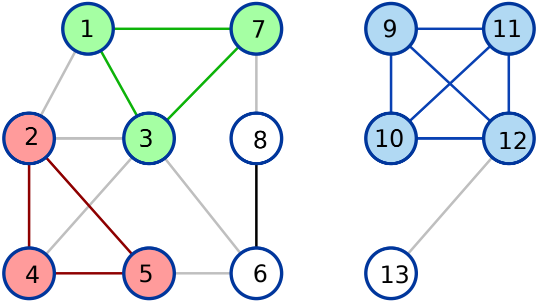

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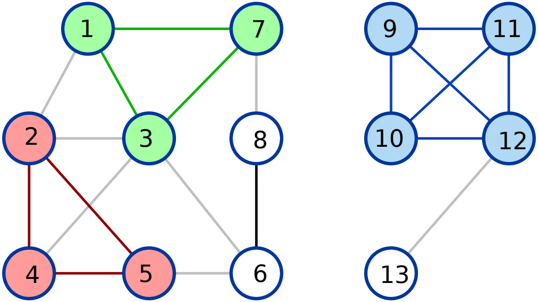

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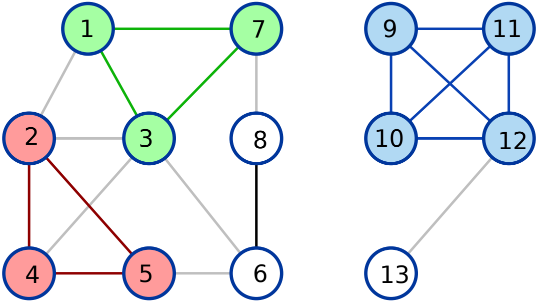

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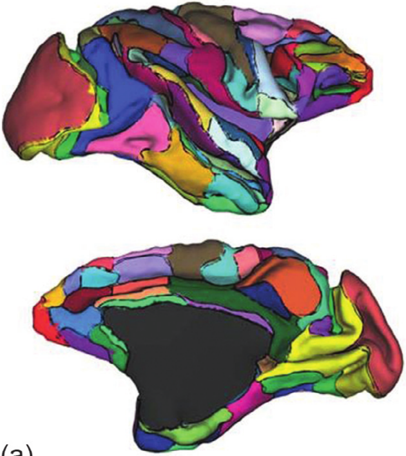
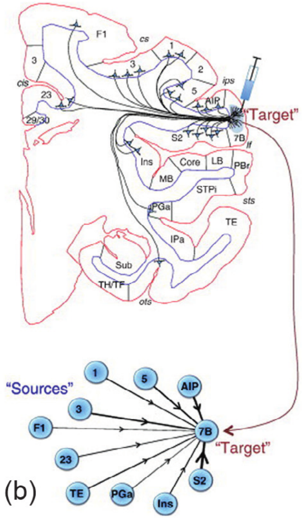
- Will every edge in G be in some clique in the decomposition? Can a node be in multiple cliques? No, to both questions.
- Modification: After finding a clique, delete only the edges in it.

Structural Connectivity at the Mesoscale


(a)

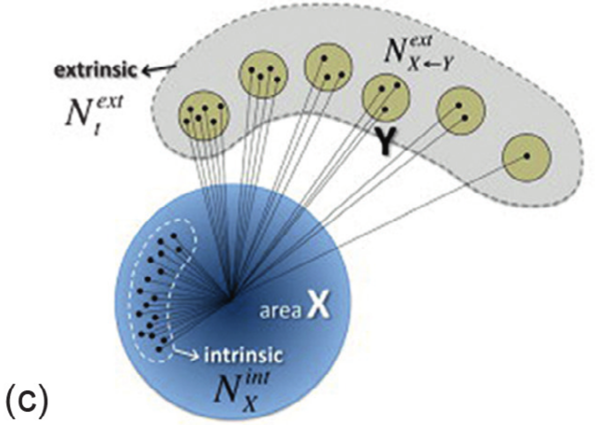
Parcellate the macaque cortex into 91 areas, defined according to cytoarchitecture and sulco-gyral landmarks.

Structural Connectivity at the Mesoscale



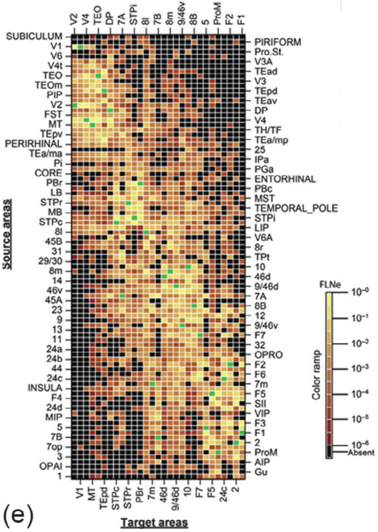
Use retrograde tract tracing. Determine edges coming into node representing area of injection from "labelled" nodes representing neurons that the tracer reaches.

Structural Connectivity at the Mesoscale



Injection is at X: $w(Y, X) = \frac{\text{number of neurons labelled in } Y}{\text{total number of labelled neurons}}$

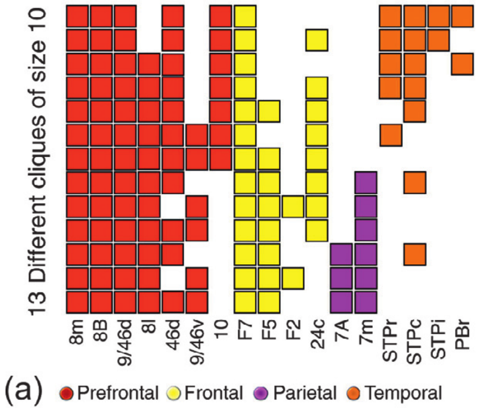
Structural Connectivity at the Mesoscale



Example of connectivity matrix.

Edge weights range over six orders of magnitude.

Cliques in Macaque Cerebral Cortex Connectome



- 29-node directed graph representing connectome of the cerebral cortex of the macaque; only considering nodes with tracer injection points.
- Computed all 13 maximum cliques, each of which had 10 nodes.

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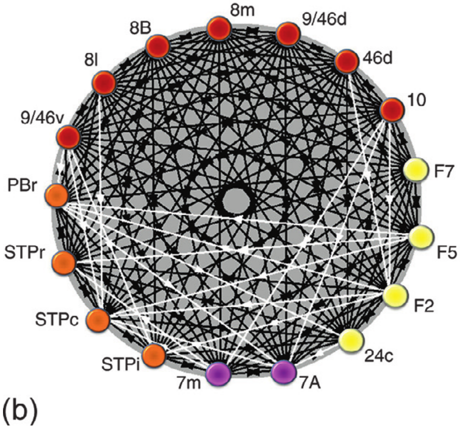
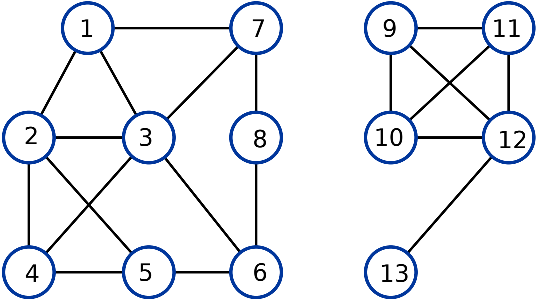


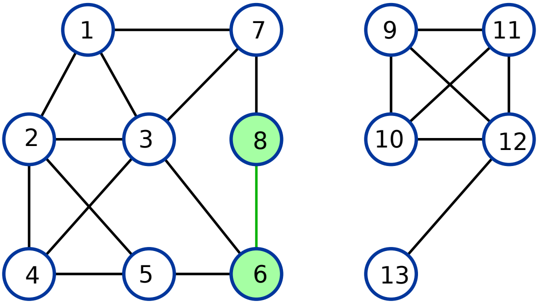
- 29-node directed graph representing connectome of the cerebral cortex of the macaque; only considering nodes with tracer injection points.
- Computed all 13 maximum cliques, each of which had 10 nodes.
- Union of cliques formed a dense subgraph among 17 nodes.

k-Cores



- In an undirected graph $G = (V, E)$, a subset of nodes $C \subseteq V$ is a *k-core* if every node $u \in C$ is connected in G to at least k nodes in C.

k-Cores



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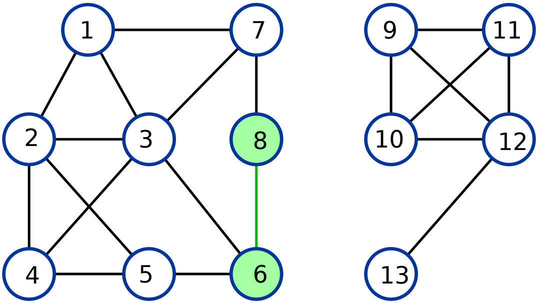

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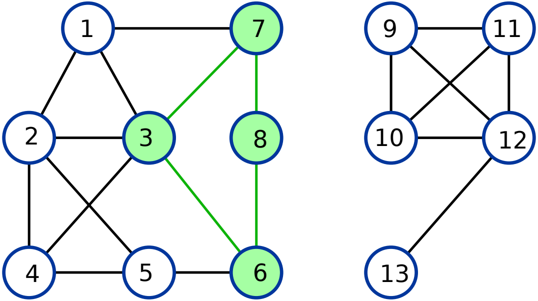
k-Cores



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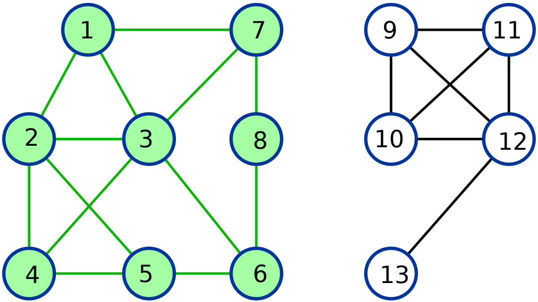

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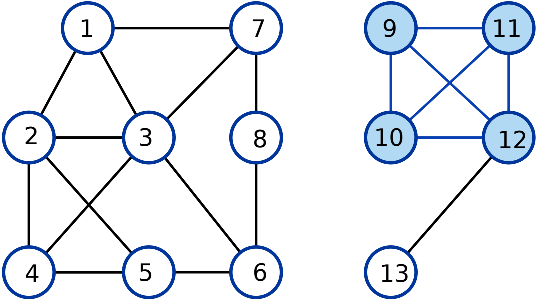

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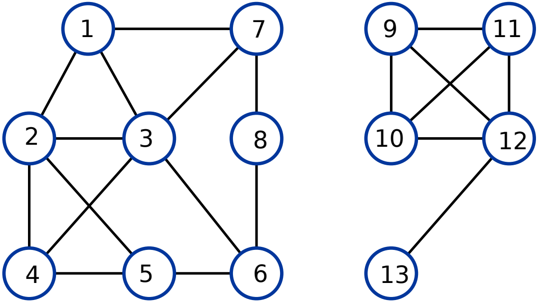
- Does this graph have a 4-core?

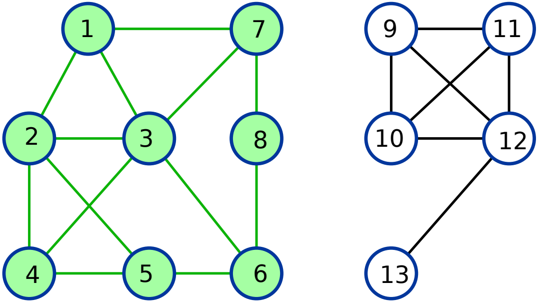
Problems related to k-cores



k-CORE EXISTENCE

Given an undirected, unweighted graph $G(V, E)$ and an integer k, compute the k-core with the largest number of nodes in G.

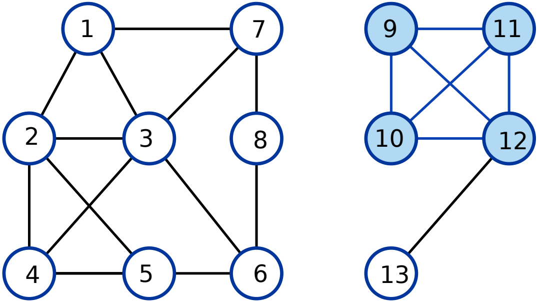
Problems related to k-cores



k-core Existence

Given an undirected, unweighted graph $G(V, E)$ and an integer k, compute the k-core with the largest number of nodes in G.

Problems related to k-cores



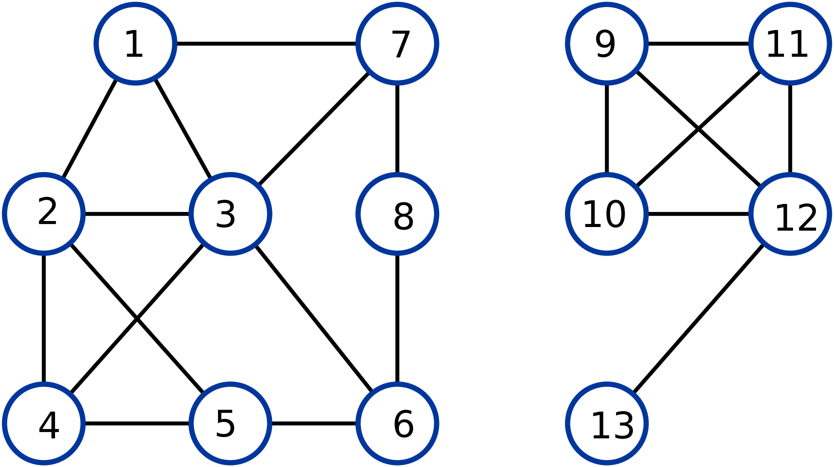
k-core Existence

Given an undirected, unweighted graph $G(V, E)$ and an integer k, compute the k-core with the largest number of nodes in G.

Largest k-core

Given an undirected, unweighted graph $G(V, E)$, compute the largest value of k for which G contains a k-core.

Algorithm for k-Core Existence



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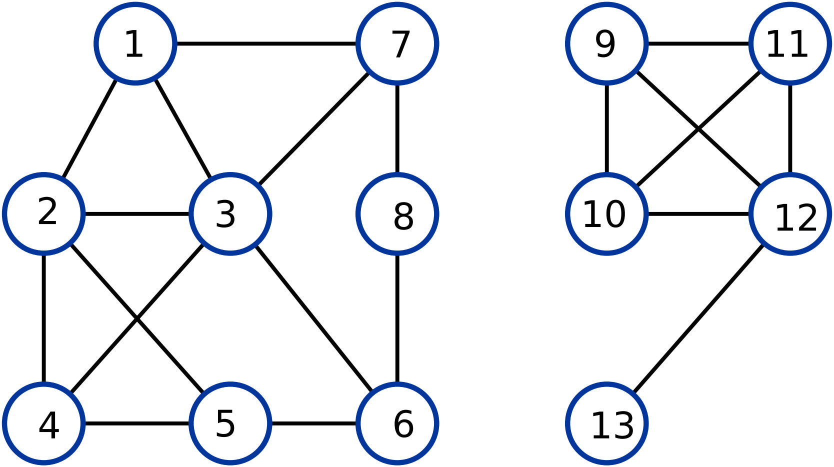

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- Resulting graph is the largest k-core.

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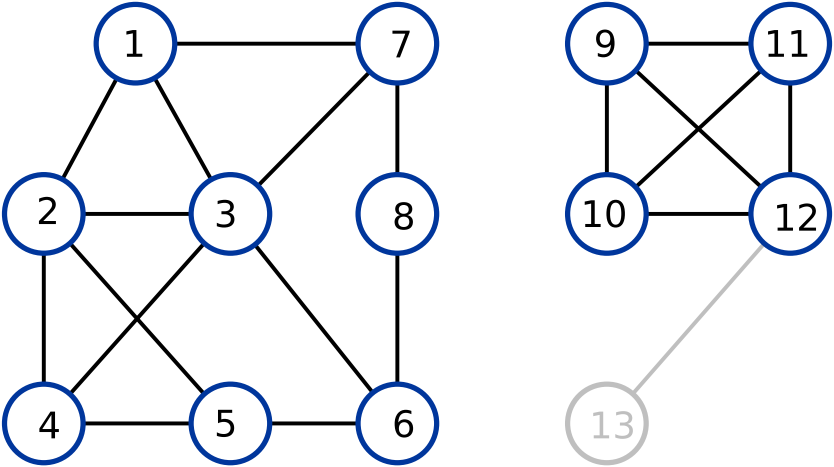

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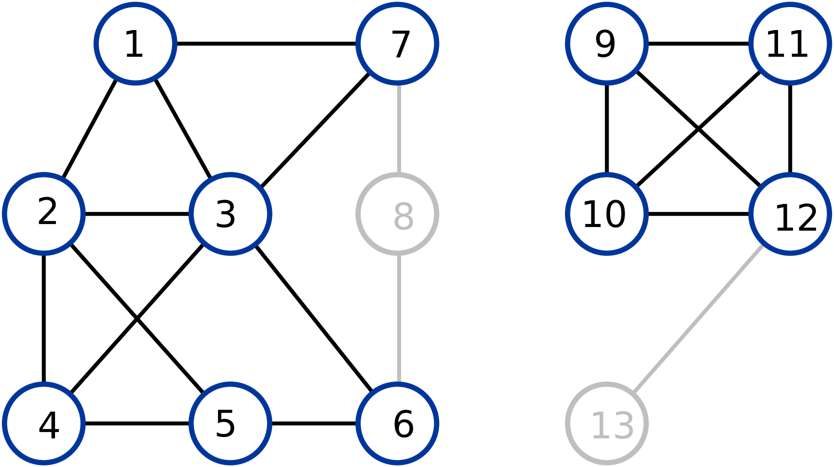

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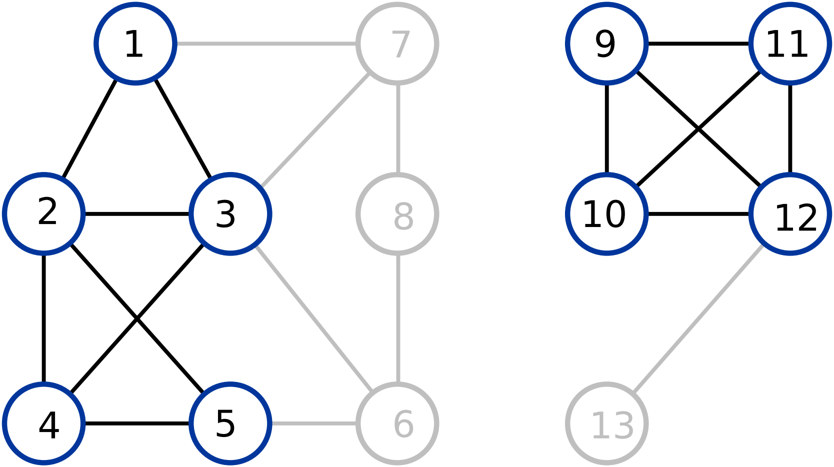

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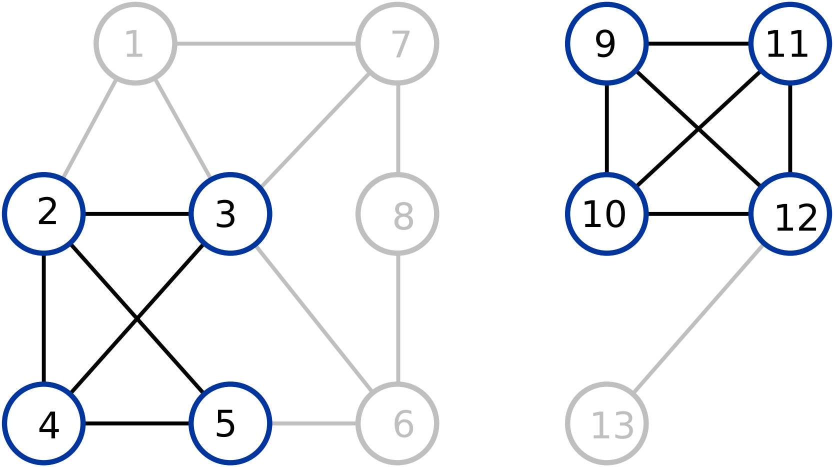

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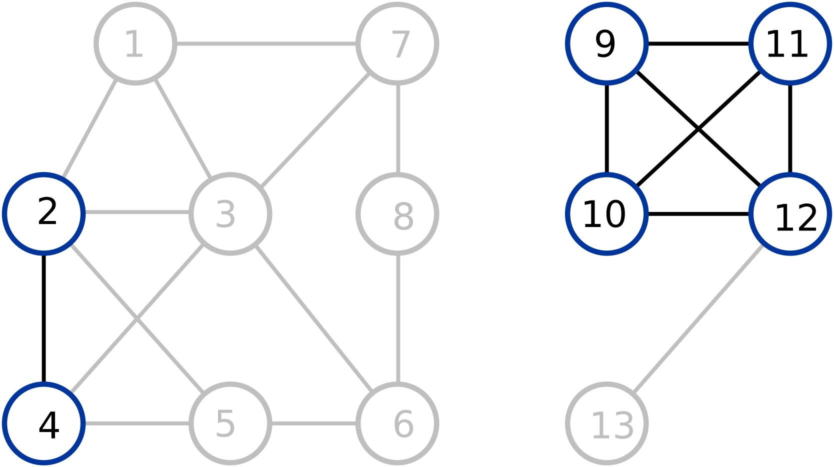

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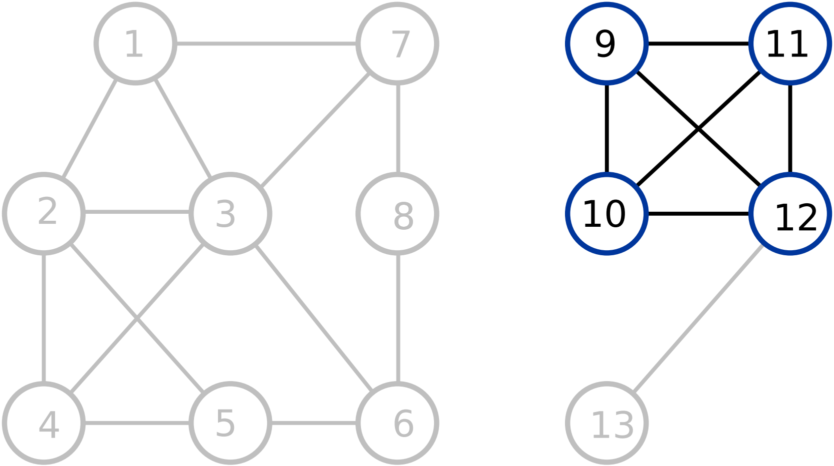

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Correctness of k-Core Existence Algorithm

- Repeatedly delete all nodes of degree $< k$ until every remaining node has degree $\geq k$.
- Why should the resulting graph H be a k-core?
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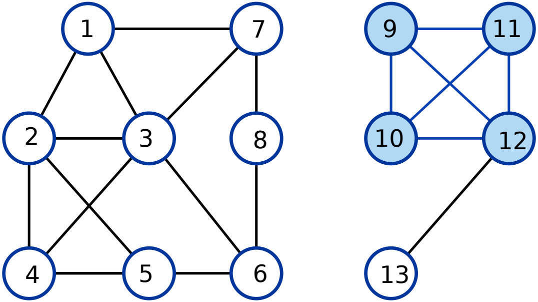
- How do we implement k-core algorithm efficiently?

Cores vs. Cliques



- A clique with k nodes is a $(k-1)$-core.
- Can we use the k-core algorithm to find maximum cliques?

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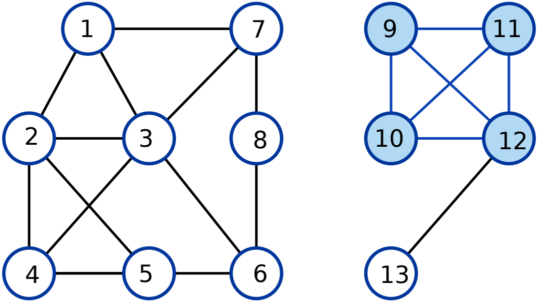

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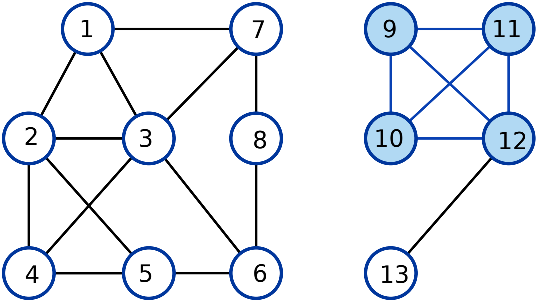

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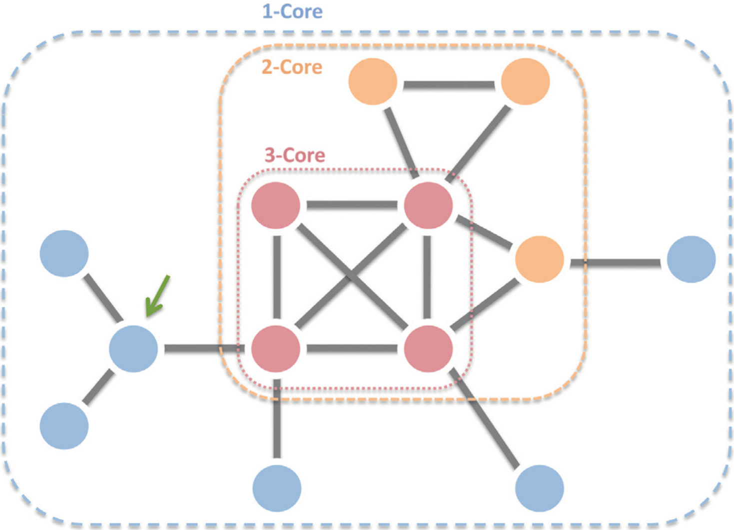
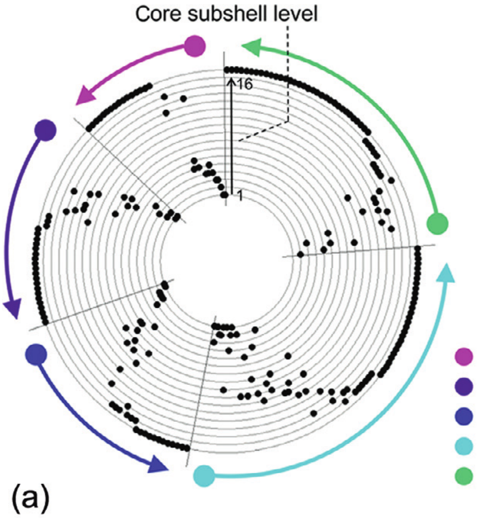
- Can we use the k-core algorithm to find maximum cliques?
- Idea: Compute the largest value of k for which a k-core H exists. If H is a clique, it must be the largest clique (of size $k+1$) in the graph.
- Flaw is that H may not be a clique, in general. The largest clique may be disjoint from H or be a subgraph of H.
- Moreover, the maximum clique may have l nodes while there may be a k-core where $k > l - 1$, e.g., $k = 3$ and $l = 3$. Create such an example.

k-Core Decomposition



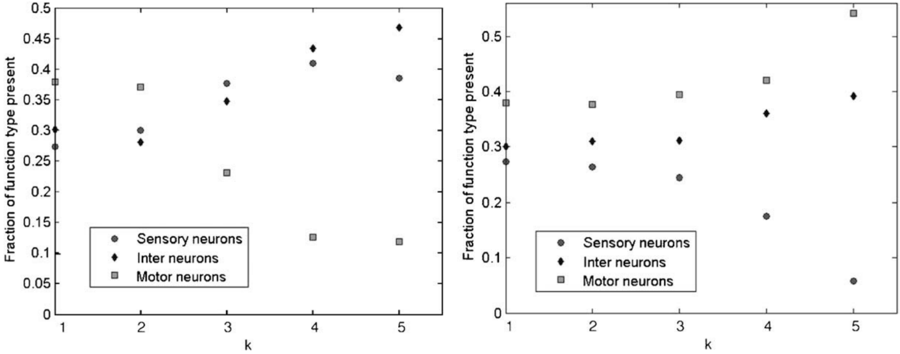
- Label each node by the k-core to which it belongs.

k-Core Decomposition of Macaque Cortex



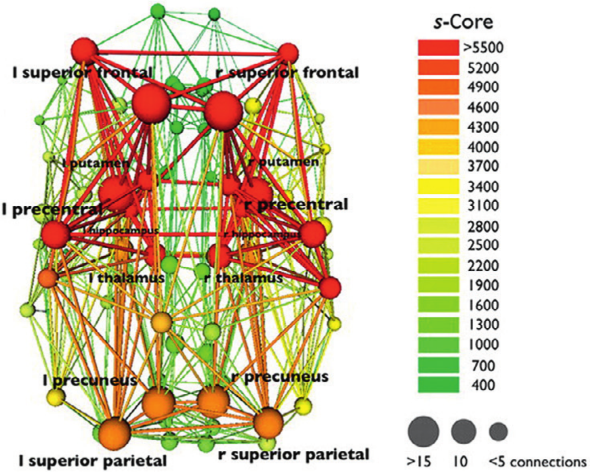
- 242-region macaque cortical connectome containing a 16-core.

k-Core Decomposition of C. Elegans Connectome



- Sensory neurons comprise the innermost cores based on out-degree.
- Motor neurons comprise the inner-most cores based on in-degree.

s-Core Decomposition of Human Connectome



- Structural connectivity from diffusion tensor imaging.
- Connectome is the average of 21 individuals.
- Extend k-core algorithm to weighted networks.