Graphs: Intro, DFS & BFS

Pedro Ribeiro

DCC/FCUP

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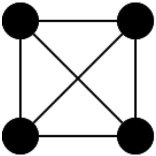
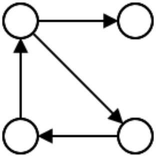
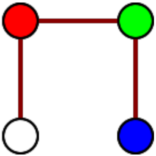
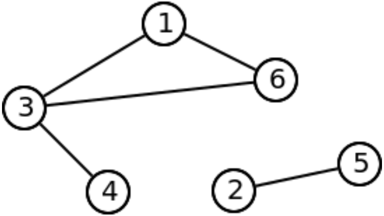




Concept

Graph Definition

Formally, a **graph** is:

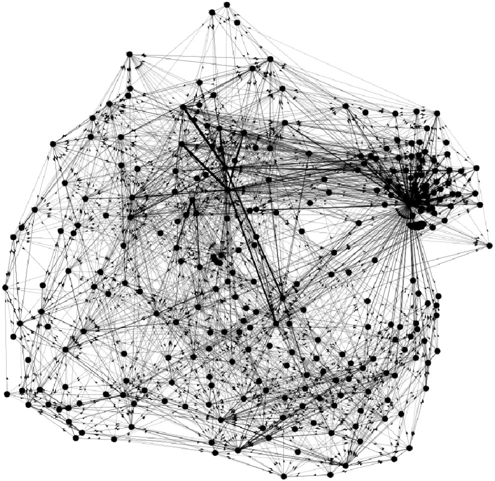
- A set of **nodes**/**vertices** (**V**).
- A set of **links**/**edges** (**E**), that connect pairs of vertices



- $V = \{1, 2, 3, 4, 5, 6\}$
- $E = \{(1, 6), (1, 3), (3, 6), (3, 4), (2, 5)\}$

What are graphs for?

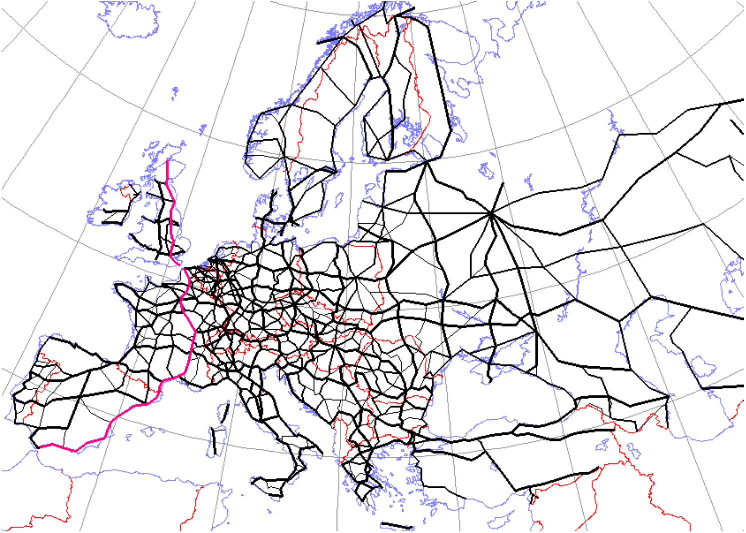
- Graphs are **ubiquitous** in Computer Science and they are present, implicitly or explicitly in many algorithms.
- They can be used in a multitude of applications.



Graph Examples

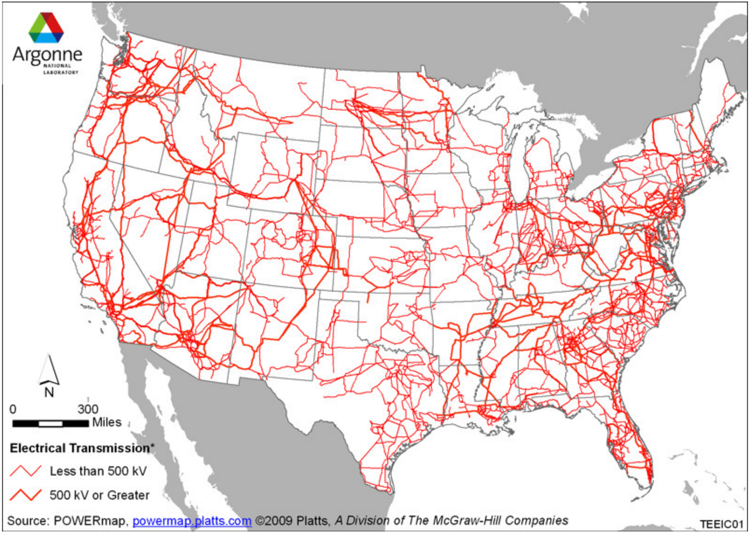
Networks that exist in the real "physical" world

- Road Network



- Public Transportation (ex: subway, train)

- Power Grid


Argonne
NATIONAL LABORATORY
N
0
300
Miles
Electrical Transmission*
Less than 500 kV
500 kV or Greater
Source: POWERmap, powermap.platts.com ©2009 Platts, A Division of The McGraw-Hill Companies
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Graph Examples

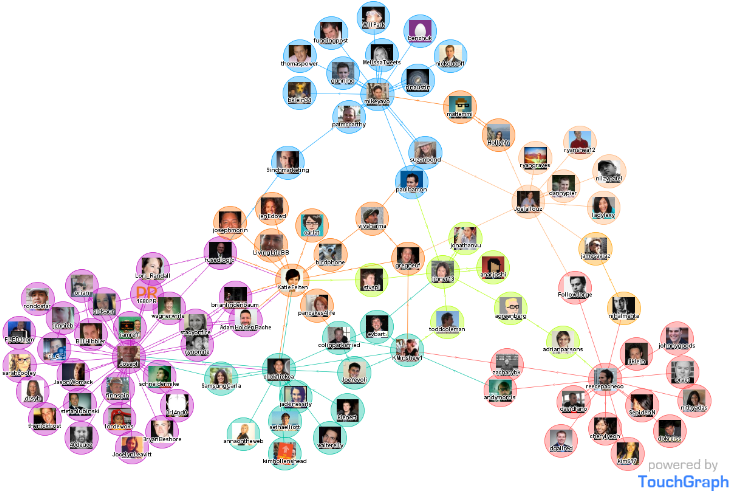
Networks that exist in the real "physical" world

- Computer Network

Graph Examples

Social Network

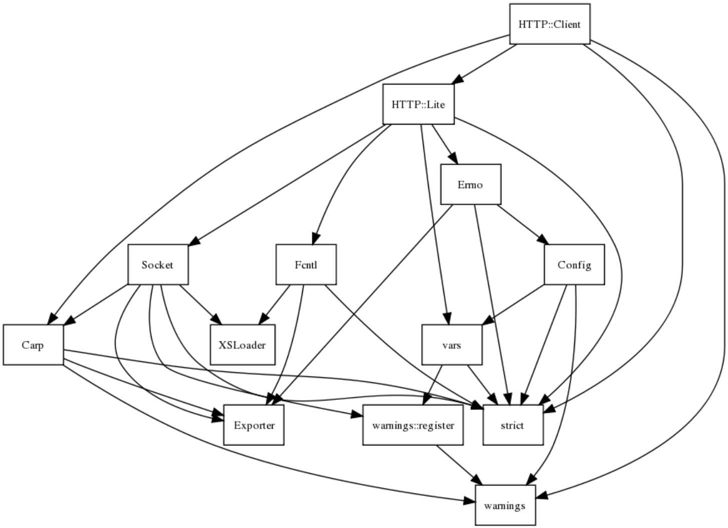
- Facebook (others: Twitter, emails, co-authorship of articles, ...)



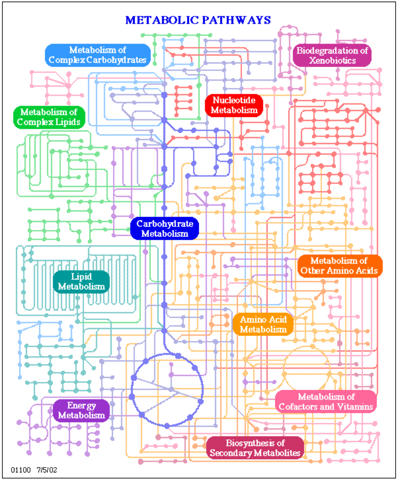
Graph Examples

Software Networks

- Module Dependencies (other examples: state, information flow, ...)

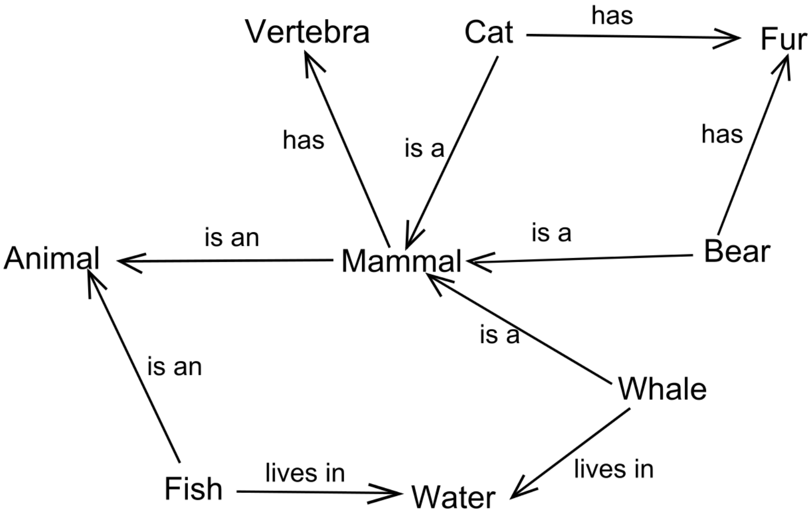


- Metabolic Networks (other examples: protein interaction, brain networks, food webs, phylogenetic trees, ...)



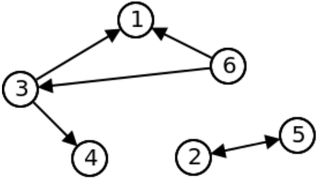
Graph Examples
Other Graphs

- Semantic Networks (other examples: world wide web, ...)

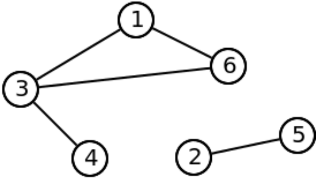


Terminology

- **Directed** graph - each link has a starting node (**origin**) and an **end** node (order matters!). Usually we use arrows to indicate the direction.
- **Undirected** graphs - There is no origin or end, but just a connection



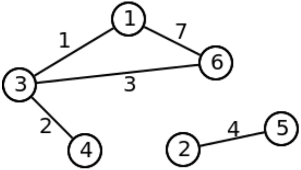
Directed Graph



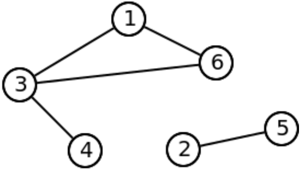
Undirected Graph

Terminology

- **Weighted** graph - there is a vale associated with each link (it could be distance, cost, ...)
- **Unweighted** - there are no weights associated with a link



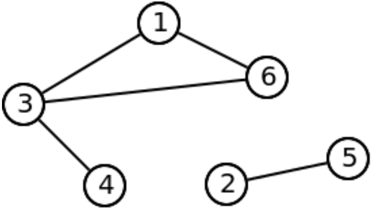
Weighted Graph



Unweighted Graph

Terminology

- **Degree** - number of connections of a node
- In directed graphs we can distinguish between **indegree** and **outdegree**



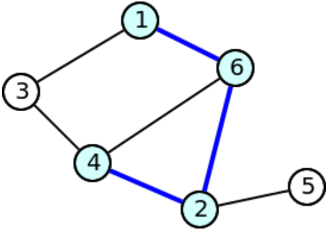
1 has degree 2
2 has degree 1
3 has degree 3
4 has degree 1
5 has degree 1
6 has degree 2

Terminology

- **Adjacent/neighbor** node: two nodes are neighbors if they are linked
- **Trivial graph**: graph with no edges and a single node
- **Self-loop**: link from a node to itself
- **Simple graph:** graph without self-loops and without repeated links (we are mostly going to work with simple graphs)
- **Multigraph:** graph with multiple links between the same node pair
- **Dense graph:** with many links when compared with the maximum possible - $|E|$ of the order of $\mathcal{O}(|V|^2)$
- **Sparse graph:** with few links when compared with the maximum possible - $|E|$ with lower order than $\mathcal{O}(|V|^2)$

Terminology

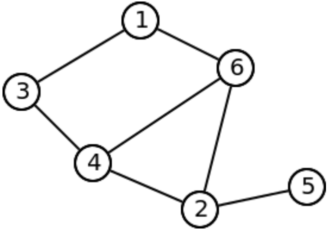
- **Path**: sequence alternating nodes and edges, such that two consecutive nodes are linked. In simple graphs we typically describe a path using just the nodes.



$1 \rightarrow 6 \rightarrow 2 \rightarrow 4$

- **Cycle**: path that starts and ends on the same node (ex: for the above graph, $1 \rightarrow 6 \rightarrow 4 \rightarrow 3 \rightarrow 1$ is a cycle)
- **Acyclic graph**: graph without cycles

- **Size** of a path: number of edges in the path
- **Cost** of a path: if the graph is weighted, we can talk about the cost, which is the sum of the edge weights
- **Distance**: size/cost of the smallest path between two nodes
- **Diameter** of a graph: max distance between two nodes of a graph



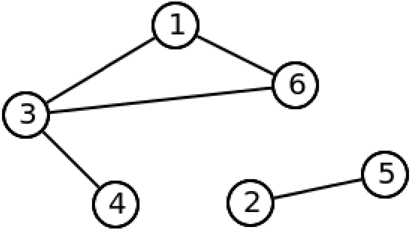
Diameter = 3

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

Distances between nodes

Terminology

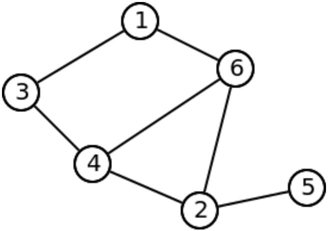
- **Connected Component**: Subset of nodes where there is at least one path between each of them
- **Connected Graph**: Graph with just one connected component (there is a path between all pairs of nodes)



Graph with two connected components: $\{1, 3, 4, 6\}$ e $\{2, 5\}$

Terminology

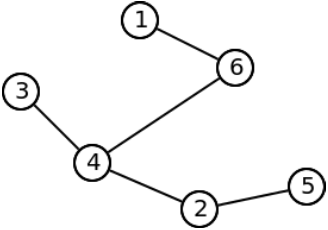
- **Subgraph**: subset of nodes and the edges between them
- **Complete** graph: with links between all pairs of nodes
- **Clique**: a complete subgraph
- **Triangle**: a clique with 3 nodes



Subgraph examples: $\{1,3\}$, $\{1,6,2\}$, $\{2,4,5,6\}$, etc
Example clique: $\{2,4,6\}$ (a triangle)

Terminology

- **Tree**: simple, connected acyclic graph
  (if it has n nodes, then it will have $n-1$ edges)
- **Forest**: set of multiple disconnected trees

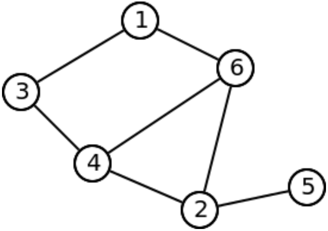


Graph Representation

How to represent a graph?

- **Adjacency Matrix**: $|V| \times |V|$ matrix where the (i, j) cell indicates if there is a link between nodes i and j (if the graph is weighted we can store the weight)

- **Adjacency list**: each node stores a list of its neighbors (if the graph is weighted we have to store pairs (destination,weight))



	1	**2**	**3**	**4**	**5**	**6**
1			X			X
2				X	X	X
3	X			X		
4		X	X			X
5		X				
6	X	X		X		

Adjacency Matrix

1: 3, 6
2: 4, 5, 6
3: 1, 4
4: 2, 3, 6
5: 2
6: 1, 2, 4

Adjacency List

Graph Representation

Some pros and cons:

- **Adjacency Matrix**:
  - Very simple to implement
  - Quick to check if there is a connection between two nodes - $\mathcal{O}(\mathbf{1})$
  - Slow to traverse the neighbors - $\mathcal{O}(|\mathbf{V}|)$
  - Lots of memory wasted (in sparse graphs) - $\mathcal{O}(|\mathbf{V}|^\mathbf{2})$
  - Weighted graph implies simply to store the weight in the matrix
  - Adding/Removing edges is simply changing a cell - $\mathcal{O}(\mathbf{1})$

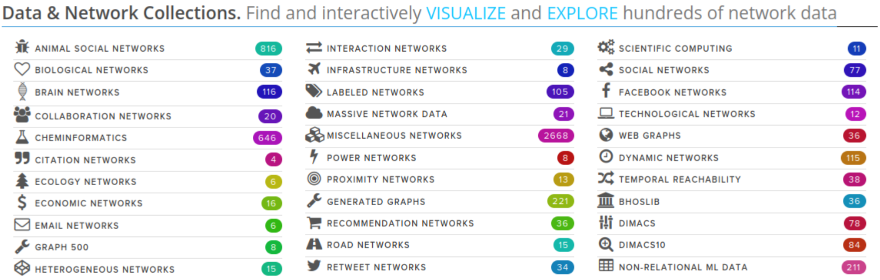
- **Adjacency List**:
  - Slow to see if there is a link between u and v - $\mathcal{O}(\mathbf{degree(u)})$
  - Quick to traverse the neighbors - $\mathcal{O}(\mathbf{degree(u)})$
  - Efficient usage of memory - $\mathcal{O}(|\mathbf{V}| + |\mathbf{E}|)$
  - Weighted graph implies adding an attribute to the list
  - Removing edge (u, v) implies traversing the list - $\mathcal{O}(\mathbf{degree(u)})$

    Note: we can use for instante BSTs (set/map) to improve the efficiency of searching and removing to $\mathcal{O}(\log degree(u))$

Graph datasets

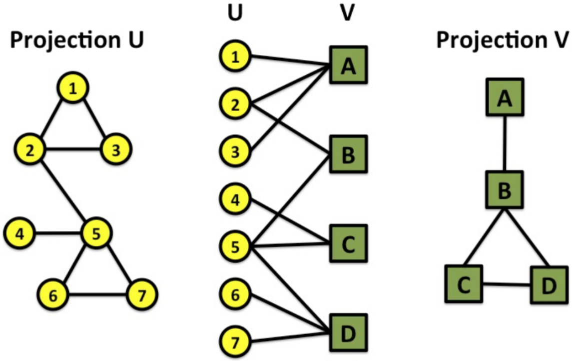
Here are some interesting websites with graphs

- **Network Repository:** `http://networkrepository.com/`
- **Konect:** `http://konect.cc/`
- **SNAP:** `https://snap.stanford.edu/data/`



Bipartite Graphs

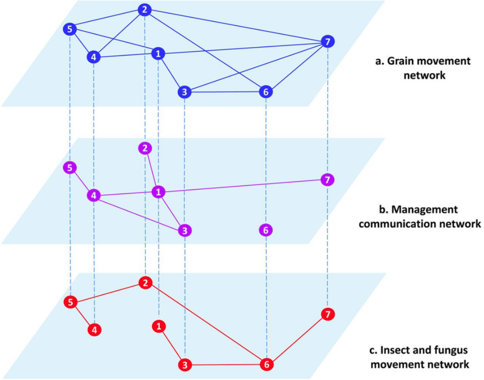
- A **bipartite graph** is a graph whose nodes can be divided into two disjoint sets U and V such that every edge connects a node in U to one in V



- Many (real world) networks come from projections (ex: actors and movies, diseases and genes)

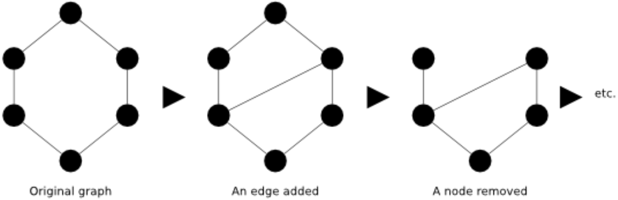
Other Graph Types: Multilayer / Multiplex

- Graphs can have different layers



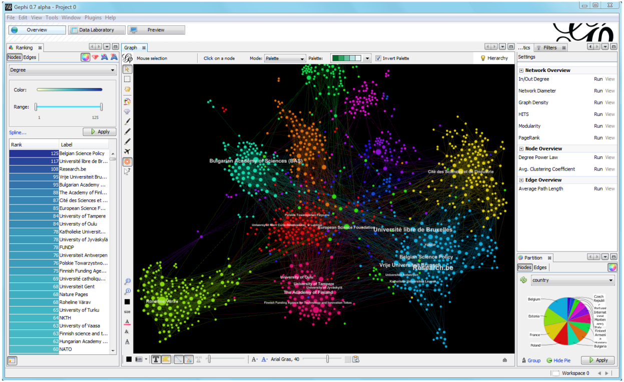
Other Graph Types: Temporal Networks

- Graphs can evolve over time



Extra: Graph Software (not needed for this course)

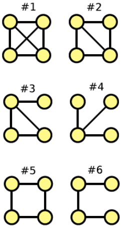
- Software such as **Gephi** or **Cytoscape** would allow you to visualize (and interact) with graphs

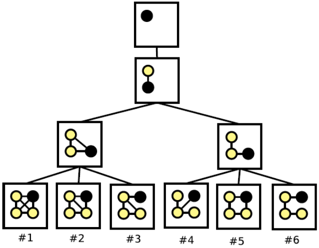


- Software packages such as **networkx** (Python) or **igraph** (C/C++, R, Python, Mathematica) provide graph implementations and many metrics and algorithms (they are *Network Science* packages)

Network Science / Graph Mining

My main research area





PhD Thesis (2011):

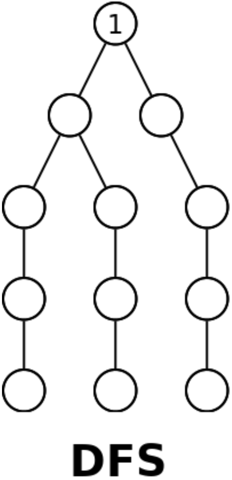
Efficient and Scalable Algorithms for Network Motifs Discovery

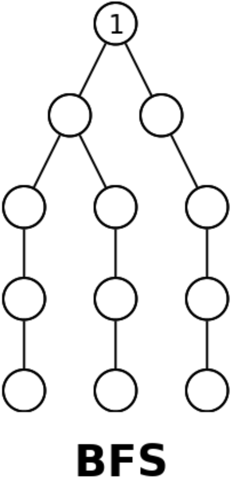
Publications: `http://www.dcc.fc.up.pt/~pribeiro/pubs_by_year.html`

Graph Traversal

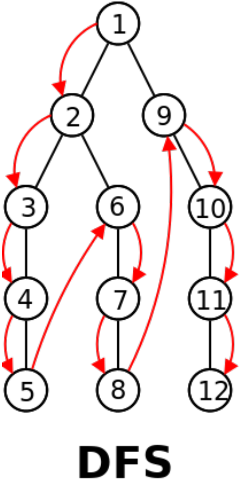
- One of the most important tasks is to **traverse** a graph, that is, **pass trough all its nodes** using the existing **links**
- We call this **graph traversal** (or **graph search**)
- There are two basic traversal types that differ on **the order in which the nodes are traversed**:
  - **Depth-First Search - DFS**
    Traverse the entire subgraph connected to a neighbor before entering the next neighbor node
  - **Breadth-First Search - BFS**
    Traverse the nodes by increasing distance of number of links to reach them

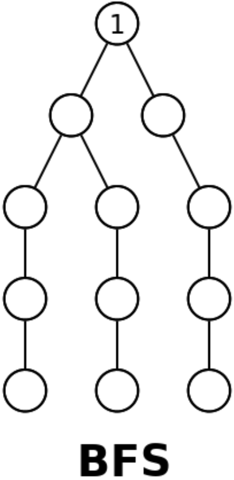
Graph Traversal



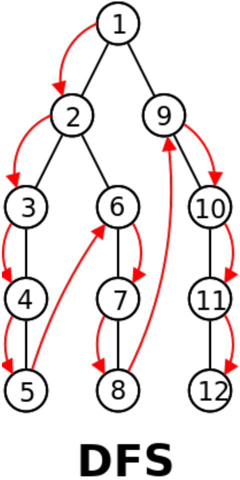


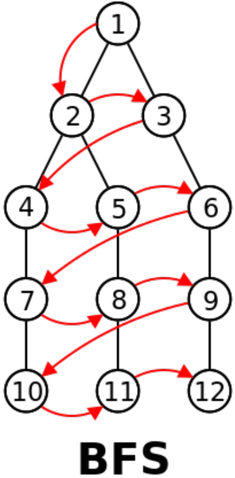
Graph Traversal





Graph Traversal





Graph Traversal

- In their essence, DFS and BFS do the "same":
  traverse all the nodes
- When to use one or the other depends on the **order that betters suits the problem** that you are solving
- Let's see how to **implement** both and give examples of applications

Depth-First Search - DFS

The "backbone" of a DFS:

DFS (recursive version)

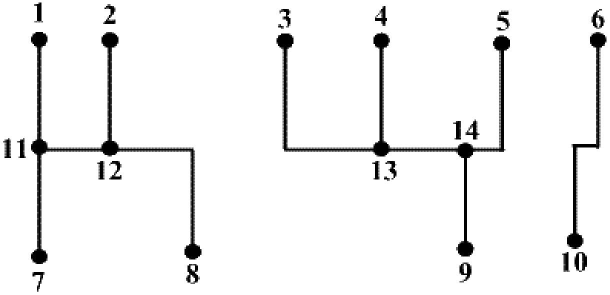
dfs(node v):
  mark v as visited
  For all neighbors w of v **do**
    If w has not yet been visited **then**
      dfs(w)

Complexity:

- Temporal:
  - Adjacency List: $\mathcal{O}(|V| + |E|)$
  - Adjacency Matrix: $\mathcal{O}(|V|^2)$
- Spatial: $\mathcal{O}(|V|)$

Example Application: Connected Components

- Find the number of **connected components** of a graph G
- Example: the following graph has **3 connected components**



Example Application: Connected Components

The "backbone" of a program to solve it:

Finding connected components

counter $\leftarrow$ 0
set all nodes as **not visited**
For all nodes v of the graph **do**
  If v has not yet been visited **then**
    counter++
    dfs(v)
write($counter$)

Temporal complexity:

- Adjacency List: $\mathcal{O}(|V| + |E|)$
- Adjacency Matrix: $\mathcal{O}(|V|^2)$

Implicit Graphs

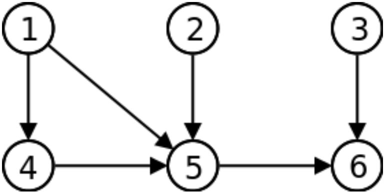
- We do not always need to explicitly store the graph
- Example: find the number of "blobs" (connected spots) in a matrix. Two cells are adjacent if they are connected vertically or horizontally.

```
#.##..##                          1.22..33
#.....##                          1.....33
...##...     -->  4 blobs  -->    ...44...
...##...                          ...44...
```

- To solve we simply need to do $dfs(x, y)$ to visit the cell (x, y) where the neighbors are $(x+1, y), (x-1, y), (x, y+1)$ and $(x, y-1)$
- Using DFS to "color" the connected components is known as doing a **Flood Fill**.

Topological Sorting

- Given a DAG G (directed acyclic graph), find an order of nodes such that u comes before v if and only if there is no edge (v, u)
- Example: For the graph below a possible topological sorting would be: $1, 2, 3, 4, 5, 6$ (or $1, 4, 2, 5, 3, 6$ - there are other possible valid orders)



A classic example of application is to decide in which order to execute a set of tasks with precedences.

Topological Sorting

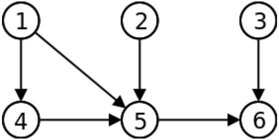
- How to solve this problem with DFS? What is the relationship between topological sorting and the DFS node order?

Topologic Sorting - $\mathcal{O}(|V| + |E|)$ (list) or $\mathcal{O}(|V|^2)$ (matrix)

order $\leftarrow$ empty
set all nodes as **not visited**
For all nodes v of the graph **do**
  If v has not yet been visited **then**
    dfs(v)
write(*order*)

dfs(node v):
  mark v as visited
  For all neighbors w of v **do**
    If w has not yet been visited **then**
      dfs(w)
  add v to the begginning of *order*

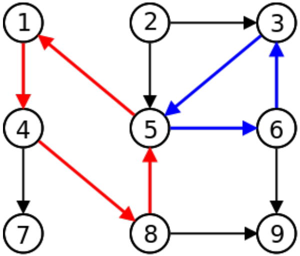
Topologic Sorting



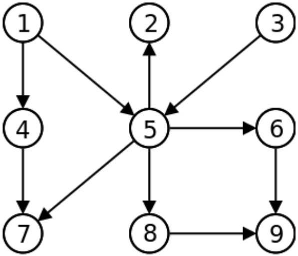
Example of execution:

- $order = \emptyset$
- start dfs(1) | $order = \emptyset$
- start dfs(4) | $order = \emptyset$
- start dfs(5) | $order = \emptyset$
- start dfs(6) | $order = \emptyset$
- end dfs(6) | $order = 6$
- end dfs(5) | $order = 5, 6$
- end dfs(4) | $order = 4, 5, 6$
- end dfs(1) | $order = 1, 4, 5, 6$
- start dfs(2) | $order = 1, 4, 5, 6$
- end dfs(2) | $order = 2, 1, 4, 5, 6$
- start dfs(3) | $order = 2, 1, 4, 5, 6$
- end dfs(3) | $order = 3, 2, 1, 4, 5, 6$
- $order = 3, 2, 1, 4, 5, 6$

- Find if a (directed) graph G us **acyclic**
- Example: the left graph has a cycle; the right graph doesn't



Graph with cycles



Acyclic Graph

Cycle Detection

Let's use 3 "colors":

- **White** - node visited node
- **Gray** - node being visited (we are exploring its descendants)
- **Black** - node already visited (we visited all its descendants)

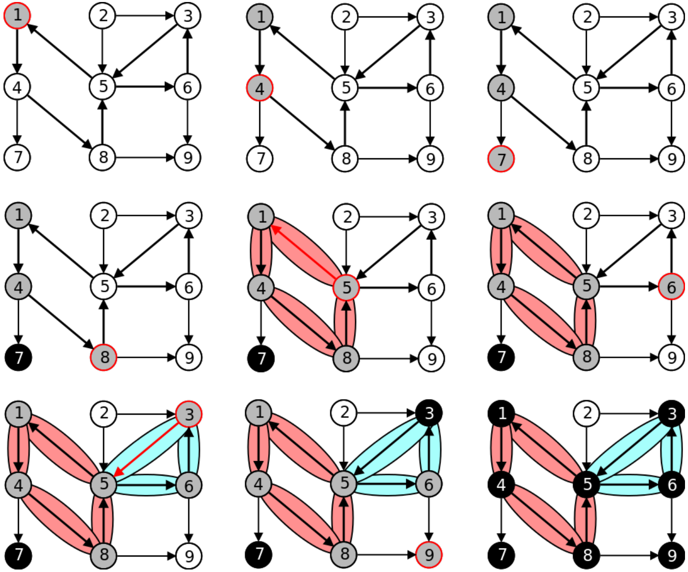
Cycle Detection - $\mathcal{O}(|V| + |E|)$ (list) or $\mathcal{O}(|V|^2)$ (matrix)

color[$v \in V$] $\leftarrow$ white
For all nodes v of the graph **do**
  If *color*[v] = white **then**
    dfs(v)

dfs(node v):
  color[v] $\leftarrow$ gray
  For all neighbors w of v **do**
    If color[w] = gray **then**
      write("Cycle found!")
    Else if color[w] = white **then**
      dfs(w)
  color[v] $\leftarrow$ black

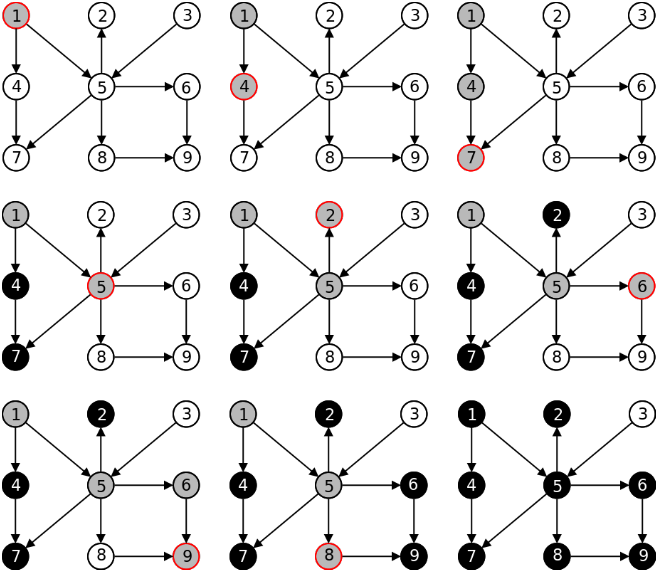
Cycle Detection

Example (starting on node 1) - graph with two cycles

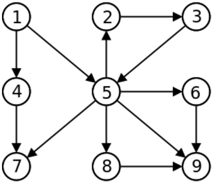


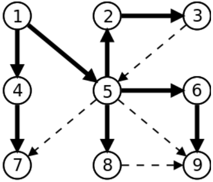
Cycle Detection

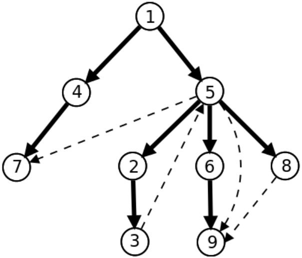
Example (starting on node 1) - acyclic graph



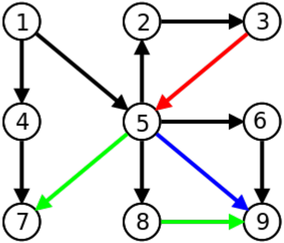
- A DFS implicitly creates a **search tree**, that corresponds to the traversed edges

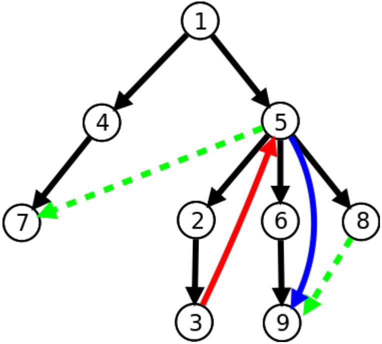






- A DFS visit separates the edges into 4 categories
  - **Tree Edges** - Edges from the DFS tree
  - **Back Edges** - Edge from a node to one of its tree ancestors
  - **Forward Edges** - Edge from a node to one of its tree descendants
  - **Cross Edges** - All other edges (from one branch to another)





Classifying DFS Edges

Another "angle" of DFS

- Example application: finding cycles is finding... **Back Edges**!
- Knowing the edge types may help to solve problem!
- Note: an undirected graph has only **Tree Edges** and **Back Edges**.

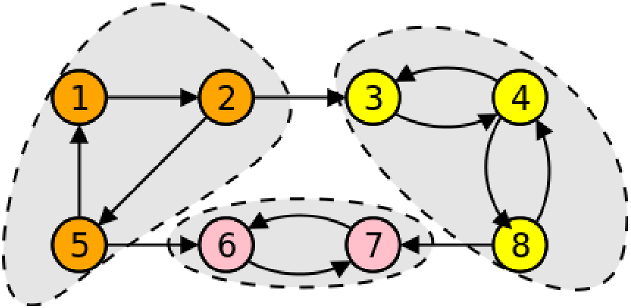
Strongly Connected Components

A more complex DFS application

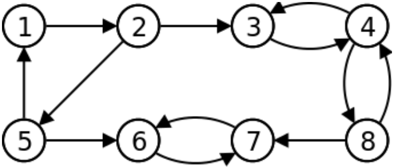
- Decompose a graph into its **strongly connected component**

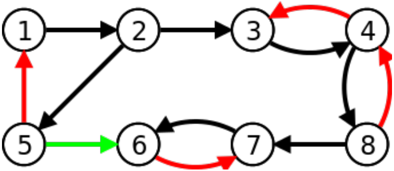
A **strongly connected component** (SCC) its a maximal subgraph where there is a (directed) path between each of its nodes.

An example graph with 3 SCCs:

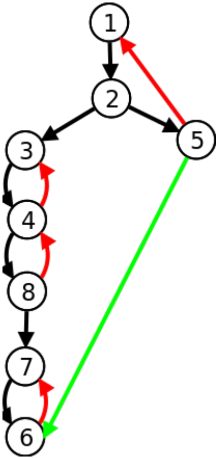


- How to compute SCCs?
- Let's try to use our knowledge about DFS edge types:





- Let's look at the generated tree:

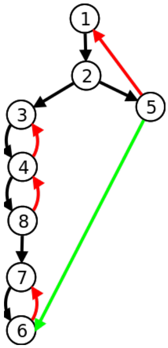


- What is the "lowest" ancestor reachable by a node?
  - 1: it's 1
  - 2: it's 1
  - 5: it's 1
  - 3: it's 3
  - 4: it's 3
  - 8: it's 3
  - 7: it's 7
  - 6: it's 7
- *Et voilà!* Here are our SCCs!

Strongly Connected Components

A more complex DFS application

- Let's add 2 attributes to the nodes in a DFS visit:
  - **num(i)**: order in which i is visited
  - **low(i)**: smallest $num(i)$ reachable by the subtree that starts in i. It's the minimum between:
    - $num(i)$
    - smallest $num(v)$ between all back edges (i, v)
    - smallest $low(v)$ between all tree edges (i, v)



i	$num(i)$	$low(i)$
1	1	1
2	2	1
3	3	3
4	4	3
5	8	1
6	7	6
7	6	6
8	5	4

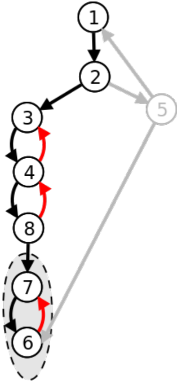
Strongly Connected Components

A more complex DFS application

Main ideas of **Tarjan Algorithm** to find SCCs:

- Make a **DFS** and in each node *i*:
  - Keep pushing the nodes to a **stack S**
  - Compute and store the values of **num(i)** and **low(i)**.
  - If when finishing the visit of a node *i* we have that **num(i)** = **low(i)**, then *i* is the "root" of a SCC. In that case, remove all the elements in the stack until reaching *i* and report those elements as belonging to a SCC!

Example of execution: in the moment we leave *dfs*(7), we find that *num*(7) = *low*(7) (7 is the "root" of a SCC)



State of Stack **S**:

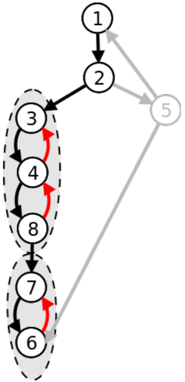
6
7
8
4
3
2
1

Remove elements from stack until reaching **7**; output SCC: {6, 7}

Strongly Connected Components

A more complex DFS application

Example of execution: in the moment we leave *dfs*(3), we find that *num*(3) = *low*(3) (3 is the "root" of a SCC)

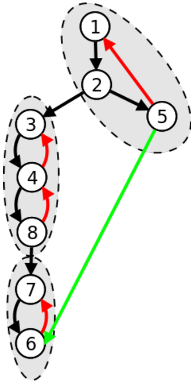


State of Stack **S**:

8
4
3
2
1

Remove elements from stack until reaching **3**; output SCC: {8, 4, 3}

Example of execution: in the moment we leave $dfs(1)$, we find that $num(1) = low(1)$ (1 is the "root" of a SCC)



State of Stack **S**:

5
2
1

Remove elements from stack until reaching **1**; output SCC:: {5, 2, 1}

Strongly Connected Components

Tarjan Algorithm for SCCs

index $\leftarrow 0$; $S \leftarrow \emptyset$
For all nodes v of the graph **do**
  If $num[v]$ is still undefined **then**
    dfs_scc(v)

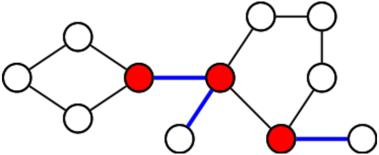
dfs_scc(node v):
  $num[v] \leftarrow low[v] \leftarrow index$; $index \leftarrow index + 1$; S.push(v)
  /* Traverse edges of v */
  For all neighbors w of v **do**
    If $num[w]$ is still undefined **then** /* Tree Edge */
      dfs_scc(w) ; $low[v] \leftarrow min(low[v], low[w])$
    Else if w is in S **then** /* Back Edge */
      $low[v] \leftarrow min(low[v], num[w])$
  /* We know that we are at the root of an SCC */
  If $num[v] = low[v]$ **then**
    Start new SCC C
    Repeat
      $w \leftarrow$ S.pop() ; Add w to C
    Until $w = v$
    Write C

Articulation Points and Bridges

An **articulation point** is a **node** whose removal increases the number of connected components.

A **bridge** is an **edge** whose removal increases the number of connected components.

Example (in red the articulation points; in blue the bridges):



A graph without articulation points is said to be **biconnected**.

Articulation Points

A more complex DFS application

- Finding **articulation points** is a very useful problem
  - For instance, a "robust" graph should not have articulation points that when "attacked" will disconnect them.
- How to compute? A possible (naive) **algorithm**:
  1. Make a DFS and count the number of connected components
  2. Remove a node from the original graph and execute a new DFS, counting again the connnected components. If this number increased, them the node is an articulation point.
  3. Repeat step 2 for all nodes in the graph
- What would be the **complexity** of this method? $\mathcal{O}(|V|(|V|+|E|))$, because we will make $|V|$ calls to DFS, each one taking $|V|+|E|$.
- **It is possible to do much better... using a single DFS**!

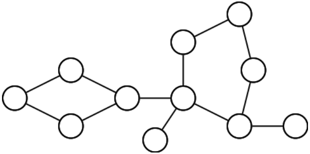
An idea:

- Apply DFS to the graph and obtain the **DFS tree**
- If a **node** v **has a child** w **without any path to an ancestor of** v**, then** v **is an articulation point**! (since removing it would disconnect w from the resto of the graph)
  - This corresponds to verify if $low[w] \geq num[v]$
- The only exception is the **root** of the DFS tree. If it has more than one child in the tree... it is also an articulation point!

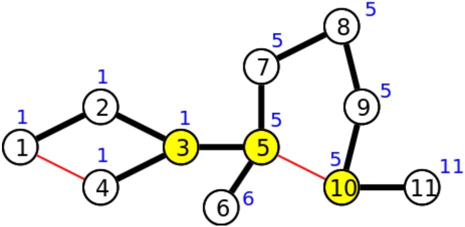
Articulation Points

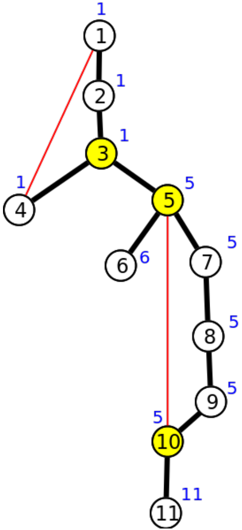
A more complex DFS application

- An example graph:



- *num*[*i*] - numbers inside the node
- *low*[*i*] - blue numbers
- articulation points: yellow nodes





- 3 is an articulation point:
  $low[5] = 5 \geq num[3] = 3$
- 5 is an articulation point:
  $low[6] = 6 \geq num[5] = 5$
  ou
  $low[7] = 5 \geq num[5] = 5$
- 10 is an articulation point:
  $low[11] = 11 \geq num[10] = 10$
- 1 is not an articulation point:
  it only has a tree edge

Articulation Points

Algorithm very similar to Tarjan, but with different DFS:

Algorithm to find articulation points

dfs_art(node v):
   $num[v] \leftarrow low[v] \leftarrow index$; $index \leftarrow index + 1$; S.push(v)
   For all neighbors w of v **do**
      If $num[w]$ is not yet defined **then** /* Tree Edge */
         dfs_art(w) ; $low[v] \leftarrow min(low[v], low[w])$
         If $low[w] \geq num[v]$ **then**
            write(v + "is an articulation point")
      Else if w is in S **then** /* Back Edge */
         $low[v] \leftarrow min(low[v], num[w])$
   S.pop()

Instead of a stack, we could have used colors (gray means it is in the stack)

Breadth-First Search - BFS

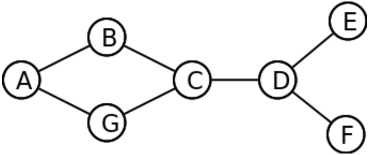
- A breadth-first search (BFS) is very similar to a DFS. It only changes the order in which the nodes are visited!
- Instead of using recursion, we will keep explicitly a queue of not visited nodes (q)

Backbone of a BFS a - $\mathcal{O}(|V| + |E|)$

bfs(node v):
   $q \leftarrow \emptyset$ /* queue of non visited nodes */
   $q.enqueue(v)$
   mark v as visited
   While $q \neq \emptyset$ /* while there are still unprocessed nodes */
      $u \leftarrow q.dequeue()$ /* remove first element of q */
      For all neighbors w of u **do**
         If w has not yet been visited **then** /* new node! */
               $q.enqueue(w)$
               mark w as visited

Breadth-First Search - BFS

- An example:



1. Initially we have $q = \{A\}$
2. We remove **A**, then we add non visited neighbors ($q = \{B, G\}$)
3. We remove **B**, then we add non visited neighbors ($q = \{G, C\}$)
4. We remove **G**, then we add non visited neighbors ($q = \{C\}$)
5. We remove **C**, then we add non visited neighbors ($q = \{D\}$)
6. We remove **D**, then we add non visited neighbors ($q = \{E, F\}$)
7. We remove **E**, then we add non visited neighbors ($q = \{F\}$)
8. We remove **F**, then we add non visited neighbors ($q = \{\}$)
9. q empty, we finished our BFS

- Almost everything than can be done with DFS can also be done with BFS!
- An important difference is that with BFS we visit the nodes in increasing order of distance (in terms of number of edges) to the initial node!
- In this way, BFS an be used to compute **shortest distances** between nodes on a **unweighted graph** (with ot without direction).
- Let's see what really changes in the code

Breadth-First Search - BFS

Computing distances

- In red the lines that were added. Em *node.distance* stores the distance to node v.

BFS - Computing distances

bfs(node v**)**:
  $q \leftarrow \emptyset$ /* Queue of non visited nodes */
  $q.enqueue(v)$
  $v.distance \leftarrow 0$ /* distance from v to itself it's zero */
  mark v as visited
  While $q \neq \emptyset$ /* while there are still unprocessed nodes */
    $u \leftarrow q.dequeue()$ /* remove first element of q */
    For all neighbors w of u **do**
      If w has not yet been visited **then** /* new node */
        $q.enqueue(w)$
        mark w as visited
        $w.distance \leftarrow u.distance + 1$

Breadth-First Search - BFS

More applications

- BFS can be applied in any graph type
- Consider for instance that you want to know the **minimum distance between** points **A** and **B** on a 2D maze:

```
########                             ########
#A.....#                             #A12345#
####.###           --->              ####4###
#B.....#     BFS starting in A       #876567#
########                             ########
```

  - A node is a cell (x, y)
  - Neighbors are $(x+1, y)$, $(x-1, y)$, $(x, y+1)$ e $(x, y-1)$
  - Everything ele in the BFS is the same! (time: $\mathcal{O}(rows \times cols)$)
  - To store on the queue we need to represent a coordinates pair (e.g.: struct in C, pair or class in C++, class in Java).