Graphs: Intro, DFS & BFS

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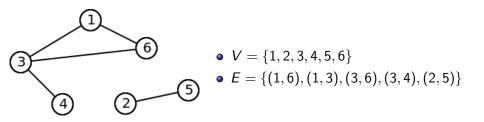


Concept

Graph Definition

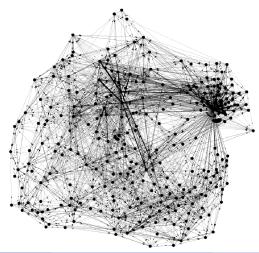
Formally, a graph is:

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



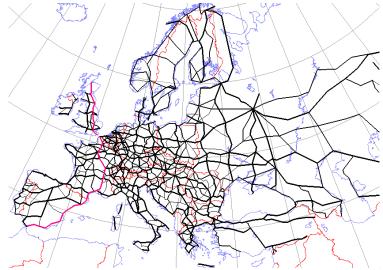
What are graphs for?

- 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.



Networks that exist in the real "physical" world

Road Network



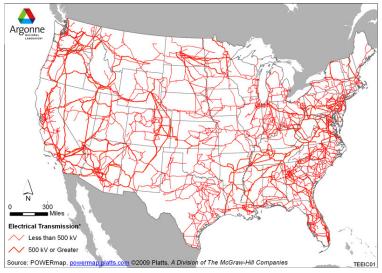
Networks that exist in the real "physical" world

• Public Transportation (ex: subway, train)



Networks that exist in the real "physical" world

• Power Grid



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Graphs: Intro, DFS & BFS

Networks that exist in the real "physical" world

• Computer Network



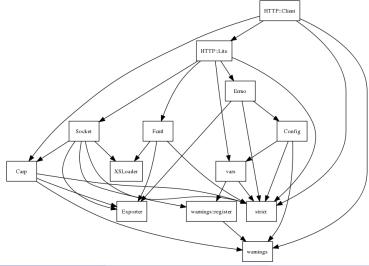
Social Network

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



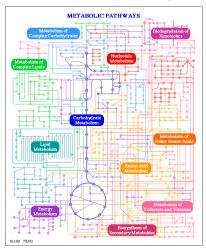
Software Networks

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



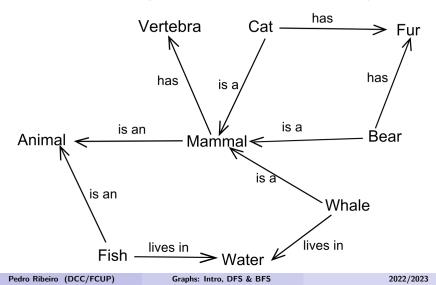
Biological Networks

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



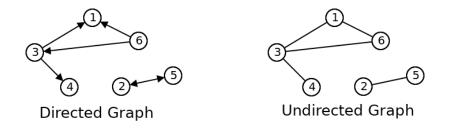
Other Graphs

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

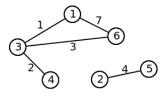


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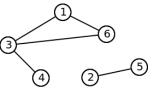
- **Directed** graph each link has a starting node (**origin**) and an **end** node (order matters!). Usually we use arrows to indicate the direction.
- Undirected graphs There is no origin or end, but just a connection



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

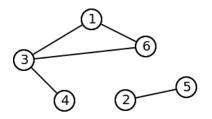


Weighted Graph



Unweighted Graph

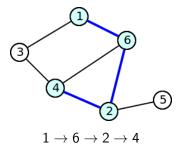
- Degree number of connections of a node
- In directed graphs we can distinguish between **indegree** and **outdegree**



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

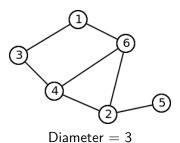
- Adjacent/neighbor node: two nodes are neighbors if they are linked
- Trivial graph: graph with no edges and a single node
- Self-loop: link from a node to itself
- Simple graph: graph without self-loops and without repeated links (we are mostly going to work with simple graphs)
- Multigraph: graph 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 $\mathcal{O}(|V|^2)$

• **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.



- **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

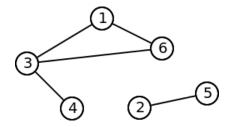
- Size of a path: number of edges in the path
- **Cost** of a path: if the graph is weighted, we can talk about the cost, which is the sum of the edge weights
- Distance: size/cost of the smallest path between two nodes
- Diameter of a graph: max distance between two nodes of a graph



	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 hotwoon nodes						

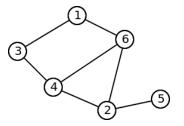
Distances between nodes

- **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)



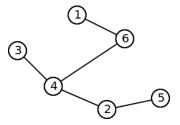
Graph with two connected components: $\{1, 3, 4, 6\} \in \{2, 5\}$

- 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



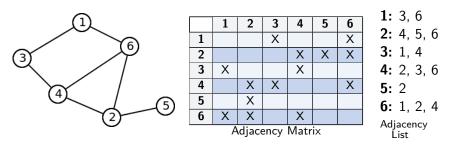
Graphs: Intro, DFS & BFS

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



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))



Graph Representation

Some pros and cons:

• Adjacency Matrix:

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

Adjacency List:

- Slow to see if there is a link between u and $v O(\text{degree}(\mathbf{u}))$
- ▶ Quick to traverse the neighbors $O(\text{degree}(\mathbf{u}))$
- ► Efficient usage of memory O(|V| + |E|)
- Weighted graph implies adding an attribute to the list
- Removing edge (u, v) implies traversing the list O(degree(u)) Note: we can use for instante BSTs (set/map) to improve the efficiency of searching and removing to O(log degree(u))

Graph datasets

Here are some interesting websites with graphs

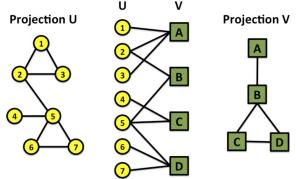
- Network Repository: http://networkrepository.com/
- Konect: http://konect.cc/
- SNAP: https://snap.stanford.edu/data/

Data & Network Collections. Find and interactively VISUALIZE and EXPLORE hundreds of network data

🕷 ANIMAL SOCIAL NETWORKS	816	INTERACTION NETWORKS	29	SCIENTIFIC COMPUTING	11
BIOLOGICAL NETWORKS	37	X INFRASTRUCTURE NETWORKS	8	SOCIAL NETWORKS	77
BRAIN NETWORKS	116	S LABELED NETWORKS	105	FACEBOOK NETWORKS	114
COLLABORATION NETWORKS	20	MASSIVE NETWORK DATA	21	TECHNOLOGICAL NETWORKS	12
	646	SMISCELLANEOUS NETWORKS	2668	WEB GRAPHS	36
55 CITATION NETWORKS	4	POWER NETWORKS	8	O DYNAMIC NETWORKS	115
ECOLOGY NETWORKS	6	PROXIMITY NETWORKS	13	C TEMPORAL REACHABILITY	38
\$ ECONOMIC NETWORKS	16	🖋 GENERATED GRAPHS	221	m BHOSLIB	36
M EMAIL NETWORKS	6	RECOMMENDATION NETWORKS	36	11 DIMACS	78
GRAPH 500	8	A ROAD NETWORKS	15	Q DIMACS10	84
HETEROGENEOUS NETWORKS	15	Y RETWEET NETWORKS	34	INON-RELATIONAL ML DATA	211

Bipartite Graphs

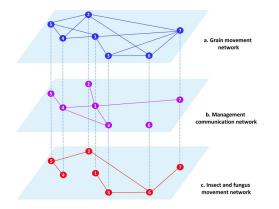
• A **bipartite graph** is a graph whose nodes can be divided into two disjoint sets *U* and *V* such that every edge connects a node in *U* to one in *V*



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

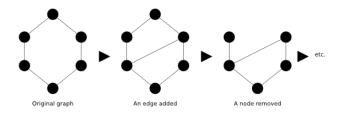
Other Graph Types: Multilayer / Multiplex

• Graphs can have different layers



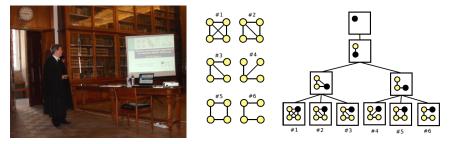
Other Graph Types: Temporal Networks

• Graphs can evolve over time



Network Science / Graph Mining

My main research area



PhD Thesis (2011): Efficient and Scalable Algorithms for Network Motifs Discovery

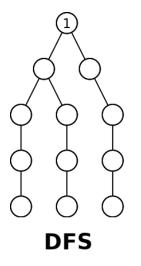
Publications: http://www.dcc.fc.up.pt/~pribeiro/pubs_by_year.html

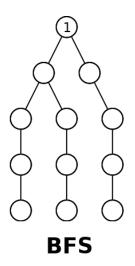
- One of the most important tasks is to traverse a graph, that is, pass trough all its nodes using the existing links
- We call this graph traversal (or graph search)
- There are two basic traversal types that differ on **the order in which the nodes are traversed**:
 - Depth-First Search DFS

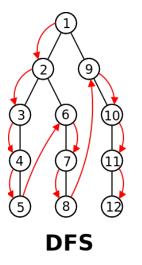
Traverse the entire subgraph connected to a neighbor before entering the next neighbor node

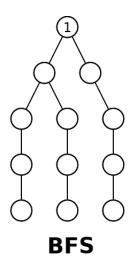
Breadth-First Search - BFS

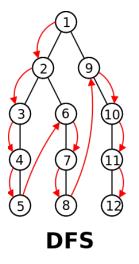
Traverse the nodes by increasing distance of number of links to reach them

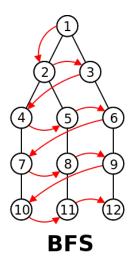












- In their essence, DFS and BFS do the "same": traverse all the nodes
- When to use one or the other depends on the **order that betters suits the problem** that you are solving
- Let's see how to implement both and give examples of applications

Depth-First Search - DFS

The "backbone" of a DFS:

DFS (recursive version)

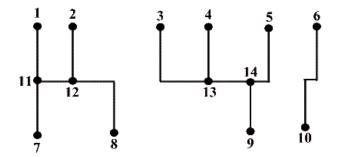
Complexity:

- Temporal:
 - ► Adjacency List: O(|V| + |E|)
 - ► Adjacency Matrix: $O(|V|^2)$

• 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(contador)
```

Temporal complexity:

- Adjacency List: O(|V| + |E|)
- Adjacency Matrix: $O(|V|^2)$

Implicit Graphs

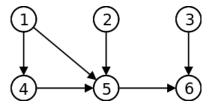
- We do not always need to explicitly store the graph
- Example: find the number of "blobs" (connected spots) in a matrix. Two cells are adjacent if they are connected vertically or horizontally.

#.####		1.22.33
###		133
##	> 4 blobs>	
##		

- 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.

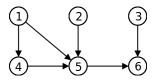
Topological Sorting

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

```
Topologic Sorting - O(|V| + |E|) (list) or 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
```

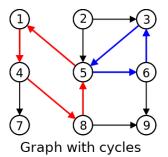
Topologic Sorting

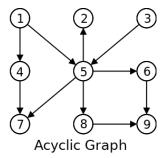


Example of execution:

• 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





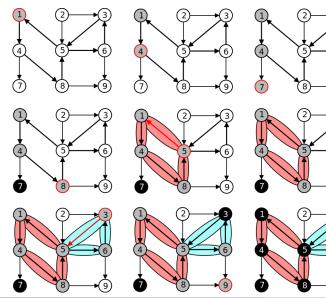
Let's use 3 "colors":

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

Cycle Detection - O(|V| + |E|) (list) or $O(|V|^2)$ (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
```

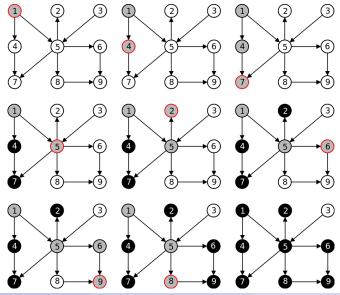
Example (starting on node 1) - graph with two cycles



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Example (starting on node 1) - acyclic graph

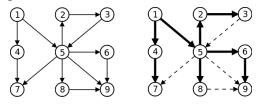


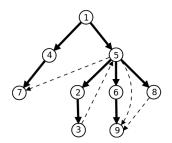
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Classifying DFS Edges

Another "angle" of DFS

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

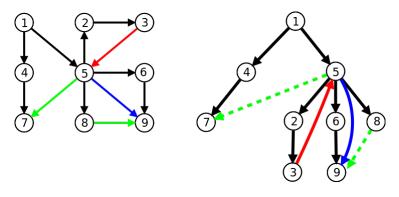




Classifying DFS Edges

Another "angle" of DFS

- 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

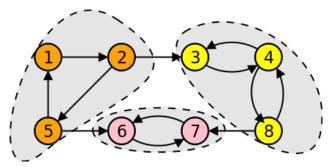
- Example application: finding cycles is finding... Back Edges!
- Knowing the edge types may help to solve problem!
- Note: an undirected graph has only Tree Edges and Back Edges.

A more complex DFS application

• Decompose a graph into its strongly connected component

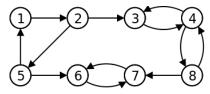
A **strongly connected component** (SCC) its a maximal subgraph where there is a (directed) path between each of its nodes.

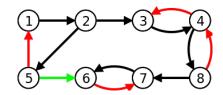
An example graph with 3 SCCs:



A more complex DFS application

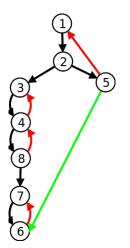
- How to compute SCCs?
- Let's try to use our knowledge about DFS edge types:





A more complex DFS application

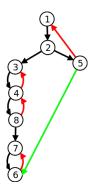
• Let's look at the generated tree:



- 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!

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

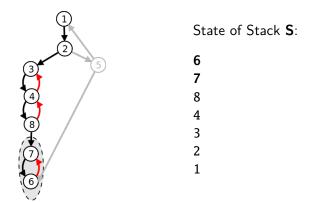
A more complex DFS application

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!

A more complex DFS application

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

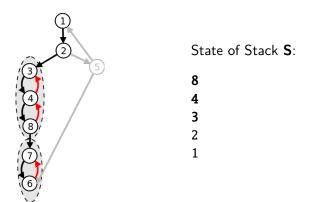


Remove elements from stack until reaching 7; output SCC: {6, 7}

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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)

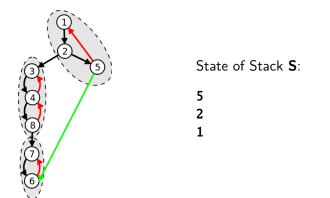


Remove elements from stack until reaching 3; output SCC: $\{8, 4, 3\}$

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A more complex DFS application

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



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

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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 \text{S.pop}(); Add w to C
     Until w = v
     Write C
```

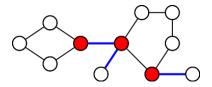
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Articulation Points and Bridges

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**.

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:
 - 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.
 - 8 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!

A more complex DFS application

An idea:

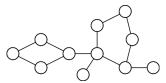
- Apply DFS to the graph and obtain the **DFS tree**
- If a node v has a child w without any path to an ancestor of v, then v is an articulation point! (since removing it would disconnect w from the resto of the graph)

► This corresponds to verify if *low*[*w*] ≥ *num*[*v*]

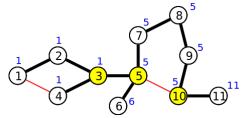
• The only exception is the **root** of the DFS tree. If it has more than one child in the tree... it is also an articulation point!

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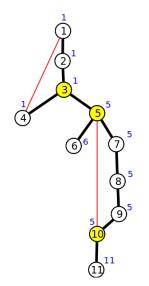
• An example graph:



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



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- 3 is an articulation point: $low[5] = 5 \ge num[3] = 3$
- 5 is an articulation point: $low[6] = 6 \ge num[5] = 5$ ou

$$low[7] = 5 \ge num[5] = 5$$

- 10 is an articulation point: $low[11] = 11 \ge num[10] = 10$
- 1 is not an articulation point: it only has a tree edge

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] \ge 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()
```

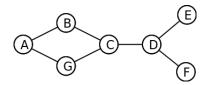
Instead of a stack, we could have used colors (gray means it is in the stack)

- 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

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• An example:



1 Initially we have $q = \{A\}$

We remove A, then we add non visited neighbors (q = {B, G})
We remove B, then we add non visited neighbors (q = {G, C})
We remove G, then we add non visited neighbors (q = {C})
We remove C, then we add non visited neighbors (q = {D})
We remove D, then we add non visited neighbors (q = {E, F})
We remove E, then we add non visited neighbors (q = {F})
We remove F, then we add non visited neighbors (q = {})
q empty, we finished our BFS

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Computing distances

- 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

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
```

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 #		# A 12345#
####.###	>	####4###
#B#	BFS starting in A	# <mark>8</mark> 76567#
#######		########

- ► 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: $O(rows \times cols)$)
- ➤ 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).

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