Graphs: Intro, DFS & BFS

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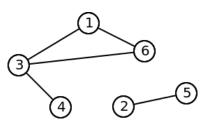


Concept

Graph Definition

Formally, a graph is:

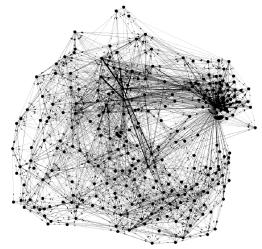
- A set of nodes/vertices (V).
- A set of links/edges (E), that connect pairs of vertices



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

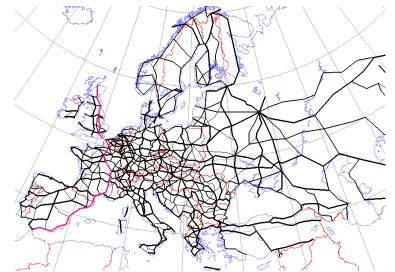
What are graphs for?

- 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.



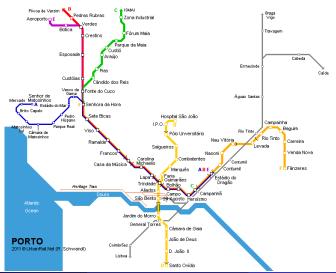
Networks that exist in the real "physical" world

Road Network



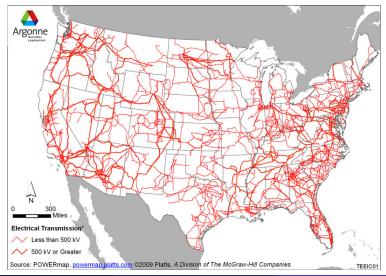
Networks that exist in the real "physical" world

• Public Transportation (ex: subway, train)



Networks that exist in the real "physical" world

Power Grid



Networks that exist in the real "physical" world

Computer Network



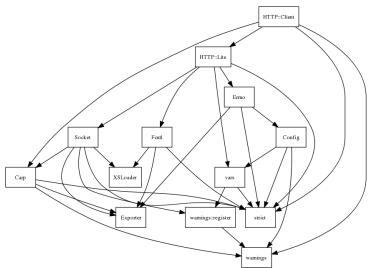
Social Network

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



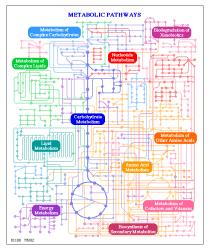
Software Networks

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



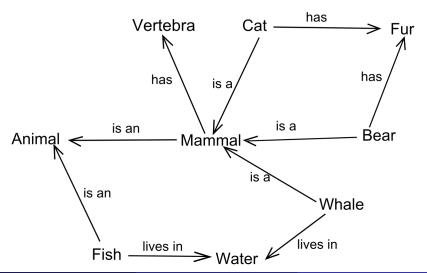
Biological Networks

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

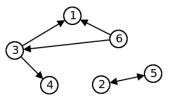


Other Graphs

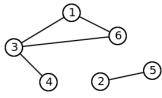
Semantic Networks (other examples: world wide web, ...)



- **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

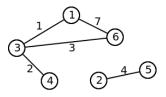


Directed Graph

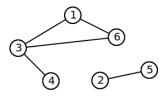


Undirected Graph

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

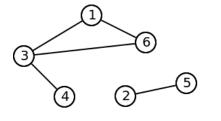


Weighted Graph



Unweighted Graph

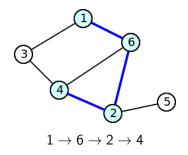
- Degree number of connections of a node
- In directed graphs we can distinguish between indegree and outdegree



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

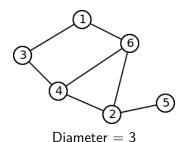
- Adjacent/neighbor node: two nodes are neighbors if they are linked
- Trivial graph: graph with no edges and a single node
- Self-loop: link from a node to itself
- Simple graph: graph without self-loops and without repeated links (we are mostly going to work with simple graphs)
- Multigraph: graph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

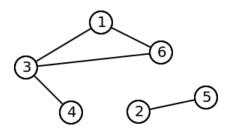
- Size of a path: number of edges in the path
- Cost of a path: if the graph is weighted, we can talk about the cost, which is the sum of the edge weights
- **Distance**: size/cost of the smallest path between two nodes
- Diameter of a graph: max distance between two nodes of a graph



	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

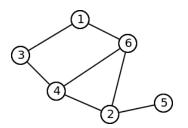
Distances between nodes

- **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)



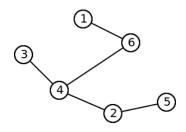
Graph with two connected components: $\{1,3,4,6\}$ e $\{2,5\}$

- 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



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

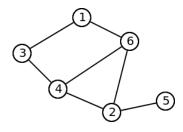
- Tree: simple, connected acyclic graph (if it has n nodes, then it will have n-1 edges)
- Forest: set of multiple disconnected trees



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			Х			Х
2				Х	Х	Х
3	Χ			Χ		
4		Х	Х			Х
5		Х				
6	Χ	Х		Х		
Adiacency Matrix						

1: 3, 6

2: 4, 5, 6

3: 1, 4

4: 2, 3, 6

5: 2

6: 1, 2, 4

Adjacency Ĺist

Graph Representation

Some pros and cons:

• Adjacency Matrix:

- Very simple to implement
- lacktriangle Quick to check if there is a connection between two nodes $\mathcal{O}(1)$
- ▶ Slow to traverse the neighbors $\mathcal{O}(|\mathbf{V}|)$
- ▶ Lots of memory wasted (in sparse graphs) $\mathcal{O}(|\mathbf{V}|^2)$
- ▶ Weighted graph implies simply to store the weight in the matrix
- lacktriangledown 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 $\mathcal{O}(\mathbf{degree}(\mathbf{u}))$
- Quick to traverse the neighbors $\mathcal{O}(\mathbf{degree}(\mathbf{u}))$
- 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 $\mathcal{O}(\text{degree}(\mathbf{u}))$ 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

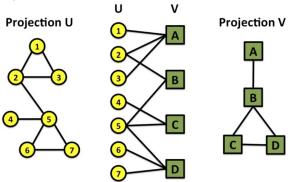
- Network Repository: http://networkrepository.com/
- Konect: http://konect.cc/
- SNAP: https://snap.stanford.edu/data/

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	★ INFRASTRUCTURE NETWORKS	8	SOCIAL NETWORKS	77
BRAIN NETWORKS	116	NABELED NETWORKS	105	f FACEBOOK NETWORKS	114
COLLABORATION NETWORKS	20	MASSIVE NETWORK DATA	21	TECHNOLOGICAL NETWORKS	12
CHEMINFORMATICS	646	& MISCELLANEOUS NETWORKS	2668	₩EB GRAPHS	36
55 CITATION NETWORKS	4	POWER NETWORKS	8	DYNAMIC NETWORKS	115
♣ ECOLOGY NETWORKS	6	PROXIMITY NETWORKS	13	▼ TEMPORAL REACHABILITY	38
\$ ECONOMIC NETWORKS	16	GENERATED GRAPHS	221	m BHOSLIB	36
EMAIL NETWORKS	6	RECOMMENDATION NETWORKS	36	TT DIMACS	78
€ GRAPH 500	8	A ROAD NETWORKS	15	€ DIMACS10	84
HETEROGENEOUS NETWORKS	15	FETWEET NETWORKS	34	■ NON-RELATIONAL ML DATA	211

Bipartite Graphs

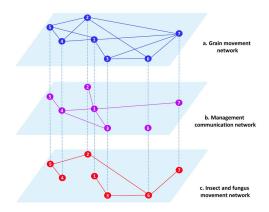
 A bipartite graph is a graph whose nodes can be divided into two disjoint sets U and V such that every edge connects a node in U to one in V



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

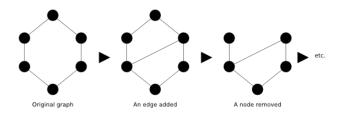
Other Graph Types: Multilayer / Multiplex

• Graphs can have different layers



Other Graph Types: Temporal Networks

• Graphs can evolve over time



Extra: Graph Software (not needed for this course)

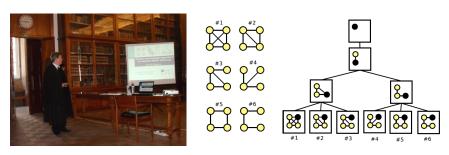
 Software such as Gephi or Cytoscape would allow you to visualize (and interact) with graphs



• 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



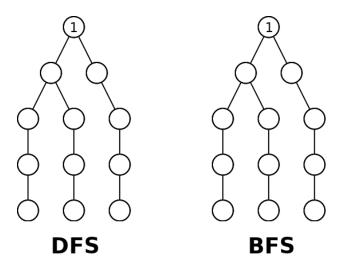
PhD Thesis (2011):

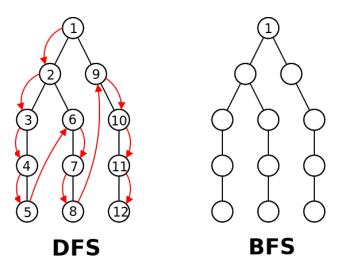
Efficient and Scalable Algorithms for Network Motifs Discovery

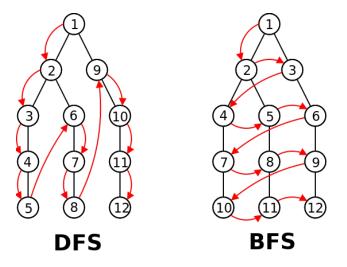
Publications: http://www.dcc.fc.up.pt/~pribeiro/pubs_by_year.html

- 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

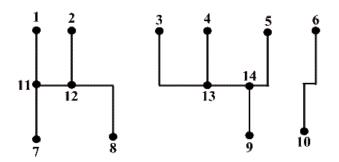
The "backbone" of a DFS:

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:

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

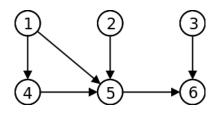
...##... --> 4 blobs --> ...44...

...##...
```

- 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)



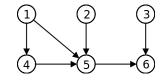
A classic example of application is to decide in which order to execute a set of tasks with precedences.

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 ← 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
```

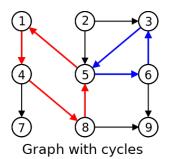
Topologic Sorting

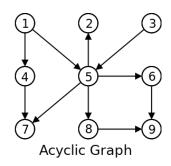


Example of execution:

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



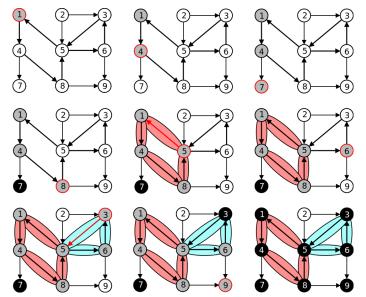


```
Let's use 3 "colors":
```

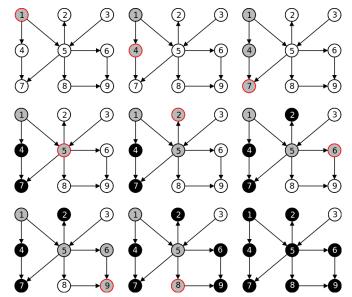
- White node visited node
- Gray node being visited (we are exploring its descendants)
- Black node already visited (we visited all its descendants)

```
Cycle Detection - \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
```

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



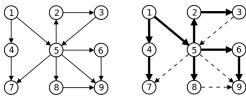
Example (starting on node 1) - acyclic graph

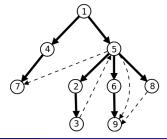


Classifying DFS Edges

Another "angle" of DFS

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

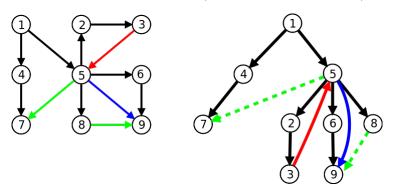




Classifying DFS Edges

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

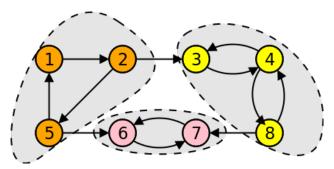
- Example application: finding cycles is finding... Back Edges!
- Knowing the edge types may help to solve problem!
- Note: an undirected graph has only Tree Edges and Back Edges.

A more complex DFS application

Decompose a graph into its strongly connected component

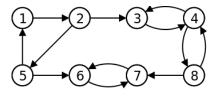
A **strongly connected component** (SCC) its a maximal subgraph where there is a (directed) path between each of its nodes.

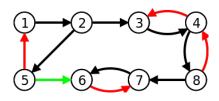
An example graph with 3 SCCs:



A more complex DFS application

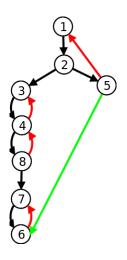
- How to compute SCCs?
- Let's try to use our knowledge about DFS edge types:





A more complex DFS application

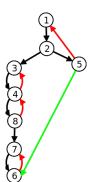
Let's look at the generated tree:



- 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
3	2	1
1	3	3
4	4	3
5	8	1
6	7	6
7	6	6
8	5	4
6 7	7	6 6

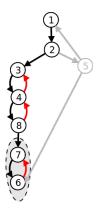
A more complex DFS application

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)

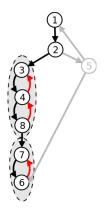


State of Stack **S**:

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

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)

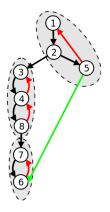


State of Stack **S**:

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

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)



State of Stack **S**:

.

1

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

```
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**.

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
 - 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!

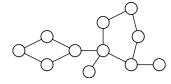
A more complex DFS application

An idea:

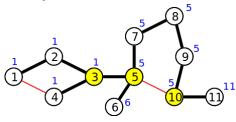
- Apply DFS to the graph and obtain the DFS tree
- If a node v has a child w without any path to an ancestor of v, then v is an articulation point! (since removing it would disconnect w from the resto of the graph)
 - ▶ This corresponds to verify if $low[w] \ge num[v]$
- The only exception is the **root**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

A more complex DFS application

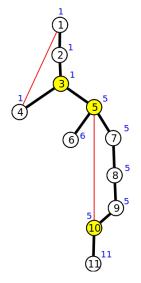
• An example graph:



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



A more complex DFS application



- 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:

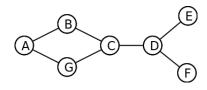
```
Algorithm to find articulation points  \begin{aligned} & \mathsf{dfs\_art}(\mathsf{node}\ v): \\ & \mathit{num}[v] \leftarrow \mathit{low}[v] \leftarrow \mathit{index}\ ; \ \mathit{index} \leftarrow \mathit{index} + 1\ ; \ \mathsf{S.push}(v) \end{aligned}  For all neighbors w of v do  \begin{aligned} & \mathsf{If}\ \mathit{num}[w]\ \mathsf{is}\ \mathsf{not}\ \mathsf{yet}\ \mathsf{defined}\ \mathsf{then}\ /^*\ \mathsf{Tree}\ \mathsf{Edge}\ ^*/\\ & \mathsf{dfs\_art}(w)\ ; \ \mathit{low}[v] \leftarrow \mathit{min}(\mathit{low}[v], \mathit{low}[w]) \end{aligned}   \begin{aligned} & \mathsf{If}\ \mathit{low}[w] \geq \mathit{num}[v]\ \mathsf{then}\\ & \mathit{write}(v+"\mathsf{is}\ \mathsf{an}\ \mathsf{articulation}\ \mathsf{point}") \end{aligned}   \begin{aligned} & \mathsf{Else}\ \mathsf{if}\ w\ \mathsf{is}\ \mathsf{in}\ S\ \mathsf{then}\ /^*\ \mathsf{Back}\ \mathsf{Edge}\ ^*/\\ & \mathit{low}[v] \leftarrow \mathit{min}(\mathit{low}[v], \mathit{num}[w]) \end{aligned}   \mathsf{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
```

• 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 $(q = \{D\})$
- **1** We remove **D**, then we add non visited neighbors $(q = \{E, F\})$
- **1** We remove **E**, then we add non visited neighbors $(q = \{F\})$
- **1** We remove **F**, then we add non visited neighbors $(q = \{\})$
- g empty, we finished our BFS

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:

- ightharpoonup 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).