## 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.



## Graph Examples

## Networks that exist in the real "physical" world

- Road Network



## Graph Examples

## Networks that exist in the real "physical" world

- Public Transportation (ex: subway, train)



## Graph Examples

## Networks that exist in the real "physical" world

- Power Grid



## 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, ...)



## Graph Examples

## Biological Networks

- 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 $\mathcal{O}\left(|V|^{2}\right)$
- Sparse graph: with few links when compared with the maximum possible - $|E|$ with lower order than $\mathcal{O}\left(|V|^{2}\right)$


## 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.

- 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


## Terminology

- 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 $=3$

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathbf{1}$ | 0 | 2 | 1 | 2 | 3 | 1 |
| $\mathbf{2}$ | 2 | 0 | 2 | 1 | 1 | 1 |
| $\mathbf{3}$ | 1 | 2 | 0 | 1 | 3 | 2 |
| $\mathbf{4}$ | 2 | 1 | 1 | 0 | 2 | 1 |
| $\mathbf{5}$ | 3 | 1 | 3 | 2 | 0 | 2 |
| $\mathbf{6}$ | 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))


|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{1}$ |  |  | $X$ |  |  | $X$ |
| 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) - $\mathcal{O}\left(|\mathbf{V}|^{2}\right)$
- 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 $v-\mathcal{O}(\operatorname{degree}(\mathbf{u}))$
- Quick to traverse the neighbors - $\mathcal{O}($ 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 - $\mathcal{O}($ 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

| ，${ }_{\text {If }}$ ANIMAL SOCIAL NETWORKS | 816 | $\ddagger$ interaction networks | 29 | 额 SCIENTIFIC Computing | （11） |
| :---: | :---: | :---: | :---: | :---: | :---: |
| O biological networks | （37） | X infrastructure networks | 8 | $\sim$ social networks | 77 |
| \＆brain networks | 116 | －Labeled networks | 105 | f FACEBOOK networks | $(114$ |
| 20\％collaboration networks | 20 | －massive network data | 21 | －technological networks | （12） |
| 【 cheminformatics | 646 | \％Miscellaneous networks | 2668 | （2）web graphs | 36 |
| 95 citation networks | （4） | 4 power networks | （8） | （－）dynamic networks | 115 |
| ＊ecology networks | 6 | （0）PROXIMITY NETWORKS | （13） | C iemporal reachability | 38 |
| \＄economic networks | 16 | c generated graphs | 221 | 亜 внозия | 36 |
| $\square$ email networks | 6 | Erecommendation networks | 36 | titimacs | 78 |
| C GRaph 500 | （8） | A road networks | 15 | Q dimacsio | 84 |
| （6）heterogeneous networks | 15 | \％retweet networks | 34 | 曲 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 $V$


Projection 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

## 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: $\mathcal{O}\left(|V|^{2}\right)$
- 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
set all nodes as not visited
For all nodes v of the graph do
    If v}\mathrm{ has not yet been visited then
        counter++
        dfs(v)
write(contador)
```

Temporal complexity:

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


## 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 $d f s(x, y)$ 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 $\mathcal{O}\left(|V|^{2}\right)$ (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 = Ø
- 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 $=3,2,1,4,5,6$


## Cycle Detection

- 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 $\mathcal{O}\left(|V|^{2}\right)$ (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 $\operatorname{color}[w]=$ 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


## 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 <br> 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:


## Strongly Connected Components

A more complex DFS application

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



## Strongly Connected Components

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!


## 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 $(i, v)$
$\star$ smallest low $(v)$ between all tree edges $(i, v)$



## 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 $\operatorname{low}(\mathbf{i})$.
- If when finishing the visit of a node $i$ we have that num( $\mathbf{i})=\operatorname{low}(\mathbf{i})$, 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!


## Strongly Connected Components

A more complex DFS application

Example of execution: in the moment we leave $d f s(7)$, we find that $\operatorname{num}(7)=\operatorname{low}(7)$ (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 $d f s(3)$, we find that num $(3)=\operatorname{low}(3)$ (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: $\{8,4,3\}$

## Strongly Connected Components

A more complex DFS application

Example of execution: in the moment we leave $d f s(1)$, we find that $\operatorname{num}(1)=\operatorname{low}(1)$ (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 }\leftarrow0;S\leftarrow
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\mathrm{ low }[v]\leftarrow\mathrm{ index ; index }\leftarrow\mathrm{ index + 1; S.push(v)
    /* Traverse edges of v*/
    For all neighbors }w\mathrm{ of v do
        If num[w] is still undefined then /* Tree Edge */
            dfs_scc(w) ; low[v]}\leftarrow\operatorname{min}(low[v],low[w]
        Else if w is in S then /* Back Edge */
            low[v]}\leftarrow\operatorname{min}(\operatorname{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\leftarrowS.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!


## Articulation Points

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 $[w] \geq n u m[v]$
- 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



## Articulation Points

## A more complex DFS application



- 3 is an articulation point: $\operatorname{low}[5]=5 \geq n u m[3]=3$
- 5 is an articulation point: $\operatorname{low}[6]=6 \geq$ num $[5]=5$
ou
$\operatorname{low}[7]=5 \geq \operatorname{num}[5]=5$
- 10 is an articulation point: $\operatorname{low}[11]=11 \geq \operatorname{num}[10]=10$
- 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\mathrm{ low }[v]\leftarrow\mathrm{ index ; index }\leftarrow\mathrm{ index +1; S.push(v)
    For all neighbors }w\mathrm{ 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\operatorname{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 $\mathbf{A}$, then we add non visited neighbors $(q=\{B, G\})$
(3) We remove $\mathbf{B}$, then we add non visited neighbors $(q=\{G, C\})$
(9) We remove $\mathbf{G}$, then we add non visited neighbors $(q=\{C\})$
(3) We remove $\mathbf{C}$, then we add non visited neighbors $(q=\{D\})$
(0) We remove $\mathbf{D}$, then we add non visited neighbors $(q=\{E, F\})$
(1) We remove $\mathbf{E}$, then we add non visited neighbors $(q=\{F\})$
(8) We remove $\mathbf{F}$, then we add non visited neighbors $(q=\{ \})$
(0) q empty, we finished our BFS


## Breadth-First Search - 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


## 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 $\mathbf{A}$ and $\mathbf{B}$ on a 2D maze:

| \#\#\#\#\#\#\#\# |  | \#\#\#\#\#\#\#\# |
| :--- | :--- | :--- |
| \#A.....\# |  | \#A12345\# |
| \#\#\#\#.\#\#\# | $--->$ | \#\#\#\#4\#\#\# |
| \#B.....\# | BFS starting in A | \#876567\# |
| \#\#\#\#\#\#\# |  | \#\#\#\#\#\#\#\# |

- A node is a cell $(x, y)$
- Neighbors are $(x+1, y),(x-1, y),(x, y+1) \mathrm{e}(x, y-1)$
- 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).

