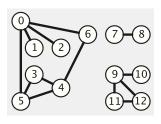
Learning from Networks

Basic Definitions and Algorithms

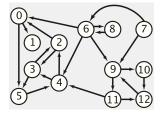
Fabio Vandin

October 2nd, 2024

Graph: Definition



Undirected graph



Directed graph

Definition

Graph G = (V, E)

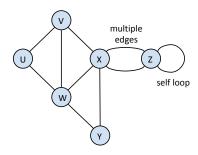
 $V \doteq$ set of vertices (sometimes called *nodes*)

 $E \doteq$ collection of edges (edge = pair of vertices).

A graph is:

- directed if every edge $(u, v) \in E$ is an ordered pair $(u \to v)$, sometimes called arc
- undirected if every edge $(u, v) \in E$ is an unordered pair (u v)

Note



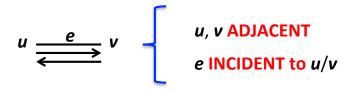
- E is a collection and not a set since there could be multiple edges u, v
- self loop: edge (u, u)
- simple graph: without multiple edges and self loops
- weighted graph: edges and/or vertices have weights

We will mostly focus on simple, unweighted graphs, but will also see some parts on weighted graphs.

Additional Terminology

Let $e = (u, v) \in E$ an edge of a graph G, then:

- e is incident to u and to v
- u and v are adjacent



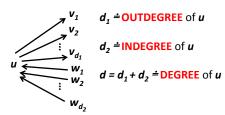
Degree

• undirected graph

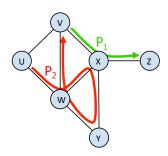


d ≐ DEGREE of u, degree(u)
num. adjacent vertices = num. incident edges

directed graph



Paths

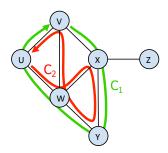


Path: sequence u_1, u_2, \dots, u_k of vertices with $(u_i, u_{i+1}) \in E$ for all $1 \le i \le k$.

Example: u, w, x, y, w, v and v, x, z are paths

Simple path: sequence u_1, u_2, \ldots, u_k of vertices all distinct with $(u_i, u_{i+1}) \in E$ for all $1 \le i < k$. Example: v, x, z is a simple path

Cycles



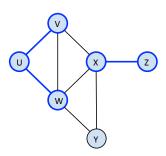
Cycle: sequence $u_1, u_2, \ldots, u_k = u_1$ of vertices with $(u_i, u_{i+1}) \in E$ for all $1 \le i < k$.

Example: $u, w, x, y, w, v, u \in v, x, y, w, u, v$ are cycles

Simple cycle: sequence $u_1, u_2, \ldots, u_k = u_1$ of vertices all distinct with $(u_i, u_{i+1}) \in E$ for all $1 \le i < k$.

Example: v, x, y, w, u, v is a simple cycle

Subgraph

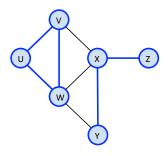


G' = (V', E') is a subgraph of G = (V, E) if:

- V' ⊂ V
 - $E' \subseteq E$
 - $\forall (u, v) \in E' : u, v \in V'$

Example: the blue edges and vertices are a subgraph of the (blue/black) graph above

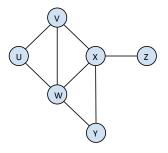
Spanning subgraph



Spanning subgraph: subgraph G' = (V', E') of G = (V, E) such that V' = V.

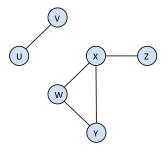
Example: the blue edges and vertices are a spanning subgraph of the (blue/black) graph above

Connected graph



G = (V, E) is connected if $\forall u, v \in V$ there exists a path in G starting in U and ending in V

Disconnected graph



G = (V, E) is disconnected if there exist $u, v \in V$ such that there is no path in G starting in U and ending in V

Connected components

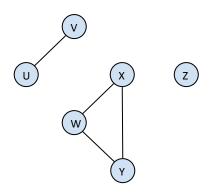
The **connected components** of G = (V, E) are a partition of G in subgraphs $\{G_1, G_2, \ldots, G_k\}$, with $G_i = (V_i, E_i)$ such that

- $G_i = (V_i, E_i)$ is connected for all $1 \le i \le k$
- $V = V_1 \cup V_2 \cup \cdots \cup V_k$ (partition of V)
- $E = E_1 \cup E_2 \cup \cdots \cup E_k$ (partition of E)
- $\forall i \neq j$ there are no edges in E between V_i and V_j

Notes:

- $\{G_i : 1 \le i \le k\}$ are maximal connected subgraphs
- if G is connected $\Rightarrow k = 1$ in the definition above
- the partition of *G* in connected components is *unique* (up to the ordering of the components)

Connected components: example



There are 3 connected components $G_1=(V_1,E_1)$, $G_2=(V_2,E_2)$, $G_3=(V_3,E_3)$ with

- $V_1 = \{u, v\} (|E_1| = 1)$
- $V_2 = \{x, y, w\} (|E_2| = 3)$
- $V_3 = \{z\} (E_3 = \emptyset)$

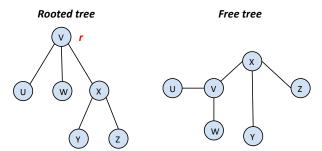
Trees

A (free) tree) is a graph G = (V, E) connected and without (simple) cycles

A **rooted tree** is a graph G = (V, E) such that:

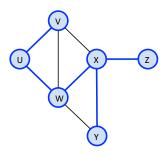
- there exist a root vertex r ∈ V
- $\forall u \in V$, with $u \neq r$, there exist a unique vertex $p(u) \in V$ parent of u
- $E = \{(u, p(u)) : u \in V, u \neq r\}$
- $\forall u \in V$ walking from parent to parent we reach r

Rooted trees vs Free trees



The concepts of *rooted tree* and of *free tree* are the *equivalent*: a rooted tree is a free tree, and vice-versa (by choosing any node as the root).

Spanning tree



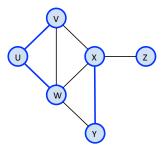
Spanning tree of *G*: connected spanning subgraph of *G* without cycles

Question: does a spanning tree exist for every **G**?

 \mathbf{No} : only if \mathbf{G} is connected

Example Edges and vertices in blue are a spanning tree of the graph above

Spanning Forest



Spanning forest of G: spanning subgraph without cycles. Example Edges and vertices in blue are a spanning forest of the graph above

Graph Properties

Let G = (V, E) be a simple and undirected graph with |V| = n and |E| = m. Then the following properties hold.

Property

$$\sum_{v \in V} degree(v) = 2m.$$

Proof

Every edge is counted twice in the sum.

Property

$$m \leq \binom{n}{2} \ (\Rightarrow m \in O(n^2))$$

Proof

Since G is simple: E is a subset of the $\binom{n}{2}$ possible pairs of vertices.

Graph Properties (continue)

Property

If G is a tree then m = n - 1

Proof

Consider G as a rooted tree. Then E contains the relations parent-child, that are n-1 (every vertex but the root has a parent).

Graph Properties (continue)

Property

If G is connected then m > n - 1

Proof

Consider the following loop:

While $(\exists \text{ cycle } C)$ do remove an edge of C from G

Then:

- at the end of every iteration: G is connected
- at the end of the loop: G is connected and without cycles, that is G is a tree with $m' = n 1 \le m$ edges.

Graph Properties (continue)

Property

If G is a forest (i.e., is without cycles) then $m \le n-1$

Proof

Consider the following loop:

While(G is not connected) do add an edge between two connected components G_1 , G_2 of G

Then:

- every added edge does not create a cycle in G;
- at the end of the loop: G is connected and without cycles, that is G is a tree with m' = n 1 > m archi.

Basic Primitives

- Graph traversal (exploration)
- Graph connectivity
- Finding connected components
- Shortest paths
- Finding a minimum spanning tree

Graph Representations: Basic Data Structures

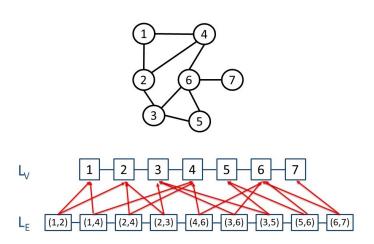
Let G = (V, E) be a graph with |V| = n and |E| = m. Note: sometimes we will assume for simplicity that $V = \{1, 2, ..., n\}$.

Simplest representation of *G* uses the following *basic data structures*:

- Vertex list L_V : every node of the list contains all relevant information for a distinct $v \in V$. If $V = \{1, 2, ..., n\}$, L_V could be an array.
- Edge list L_E : every node of the list contains all the relevant information for a distinct $e = (u, v) \in E$, including "pointers" to u and v.

Note: Depending on the problem/task, every vertex/edge can be enriched with additional information (ID, weight, labels, ecc.).

Example



Adjacency List Representation

The edge list representation L_E is not useful to develop efficient algorithms. We will now see better and commonly used representations.

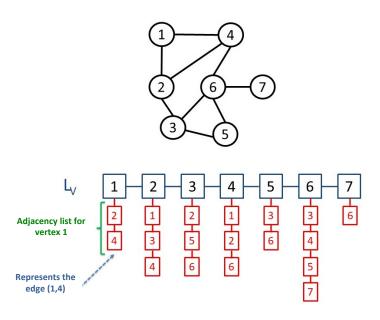
Adjacency List: For every vertex $v \in V$ there is a list I(v) of pointers to the edges (i.e., elements of L_E) incident to v.

Notes: the representation with adjacency lists is the commonly used for the following reasons:

- it allows to represent G with space linear in the size of G: $\Theta(n+m)$.
- it allows sequential access to the neighbours of a vertex v, in time linear in the degree of v (e.g., iterating on v neighbours...).

Note: we will usually assume the adjacency list representation of a graph G, and to also have L_E .

Example



Adjacency Matrix Representation

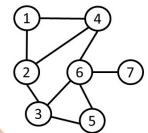
Adjacency matrix A: $n \times n$ matrix such that rows and colums are in 1 to 1 correspondence with G vertices, with

$$A[i_1, i_2] \doteq \begin{cases} null & \text{if } (i_1, i_2) \notin E \\ \text{pointer to } e = (i_1, i_2) \in L_E & \text{if such edge exists} \end{cases}$$

Notes:

- Such structure requires the vertices to be represented by integers
 (e.g., V = {1,2,...,n}) and allows O(1) (constant time) access to
 an edge and its information.
- the adjacency matrix requires space $\Theta(n^2)$, which can be superlinear in the size of G. Therefore, the representation is used mostly for *dense graphs* (number of edges roughly $\Theta(n^2)$).

Example



They represent the same edge (since the graph is undirected)

	1	2	3	4	5	6	7
1	1	(1,2)		(1,4)			
2	(2,1)		(2,3)	(2,4)			
3		(3,2)			(3,5)	(3,6)	
4	(4,1)	(4,2)				(4,6)	
5			(5,3)			(5,6)	
6			(6,3)	(6,4)	(6,5)		(6,7)
7						(7,6)	

Graph Traversal of G = (V, E)

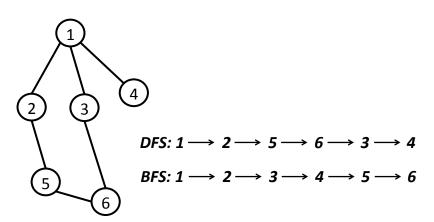
Systematic exploration of G, starting from a vertex s and visiting all vertices.

- Breadth-First Search (BFS): after visiting a vertex, visit all its neighbours before moving to the neighbours of its neighbours
- Depth-First Search (DFS): after visiting a node, visit one of its neighbours, then a neighbour of the neighbour, etc.

Note:

- Why not simply use a scan of the lists L_V e L_E?
- BFS and DFS are *design patterns*: by appropriately choosing what the "visit" of a node is, we can solve several problems: connectivity, finding a spanning tree, etc.

Example



Breadth-First Search: Algorithm BFS

- Iterative algorithm that, starting from a vertex s, "visits" all the vertices in the connected component C_s containing s, "touching" all the vertices and the edges of C_s and partitioning the vertices in levels L_i based on their distance i from s.
- Every vertex v ∈ V has a field v.ID with v.ID = 1 if v has been visited, and v.ID = 0 otherwise.
- Every edge e ∈ E has a field e.label with e.label = null if e has not been labeled yet, or it has a label between DISCOVERY EDGE or CROSS EDGE

Breadth-First Search: Algorithm BFS

Algorithm BFS(G, s)

Input: undirected graph G = (V, E), vertex $s \in V$ not visited **Output:** all the vertices of C_s are visited and all the edges C_s labeled as DISCOVERY or CROSS EDGE

Breadth-First Search: Algorithm BFS

```
visit s; s.ID \leftarrow 1;
create list L_0 containing only s; i \leftarrow 0;
while (!L_i.isEmpty()) do
    create empty L_{i+1};
    forall v \in L_i do
        forall e \in G.incidentEdges(v) do
             if (e.label = null) then
                 w \leftarrow G.opposite(v, e);
                 if (w.ID = 0) then
                      e.label ← DISCOVERY EDGE;
                     visit w;
                     w.\mathtt{ID} \leftarrow 1
                    insert w in L_{i+1};
                 else e.label ← CROSS EDGE;
return;
```

Example

Analysis of BFS

- Undirected graph $G = (V, E), s \in V$
- $C_s \subseteq G$: connected component containing s.

Proposition

Consider the execution of BFS(G,s). Assume that at the beginning, no vertex of C_s is visited and no edge of C_s is labeled. At the end of the execution:

- 1 all vertices of C_s are visited and all edges of C_s are labeled as DISCOVERY or CROSS EDGE:
- 2 the DISCOVERY EDGES are a spanning tree T of C_s rooted in s, called BFS tree;
- 3 $\forall v \in L_i$ the path in T from s to v has i edges and i is the minimum number of edges among any path from s to v in G; i is the distance between s and v;
- 4 if $(u, v) \in E$ and $(u, v) \notin T$ (\Rightarrow (u, v) is a CROSS EDGE) then the indices of $u \in V$ differ by at most 1.

Proof: see the material online.

Complexity of BFS(G, s)

Theorem

Consider the execution of BFS(G,s). Assume that at the beginning, no vertex of C_s is visited and no edge of C_s is labeled. The complexity of BFS(G,s) is Θ (m_s), where m_s is the number of edges of C_s .

Corollary

If G = (V, E) is connected, BFS(G, s) has complexity $\Theta(|E|) \forall s \in V$.

Proof of the Theorem

Visiting the Whole Graph

Note that BFS(G, s) visits only the connected component C_s of s.

How can we visit the whole graph?

This is a common *design pattern* to solve problems using the BFS.

```
forall v \in V do v.ID \leftarrow 0;
forall v \in V do
if (v.ID = 0) then
BFS(G, v);
```

Note: We assume that there is an iterator on L_V that allows to access the next vertex in time O(1).

Visiting the Whole Graph (Analysis)

Applications of BFS: Connectivity

Input: Graph G = (V, E).

Output: Number of connected components of *G* and each connected

components with a different ID values for its vertices.

Note.: If the return value is 1, then G is connected.

Let BFS(G, v, k) be a modified version of BFS(G, v), where the instruction

$$w.\mathtt{ID} \leftarrow 1$$

is substituted by

$$w.\mathtt{ID} \leftarrow k$$

The following algorithm computes the number of connected components of G and assigns to all vertices of each connected component the same value ID.

```
for v \leftarrow 1 to n do v.ID \leftarrow 0;

k \leftarrow 0;

for v \leftarrow 1 to n do

if (v.ID = 0) then

k \leftarrow k + 1;

BFS(G, v, k);
```

return k

Applications of BFS: Connectivity (Analysis)

The following proposition can be easily proved.

Proposition

Given G = (V, E), with |V| = n and |E| = m, the following problems can be solved in time O(m + n) using the BFS:

- 1 test if G is connected;
- 2 find the connected components of G;
- 3 find a spanning tree of G, if G is connected:
- 4 find a shortest path between vertices s and t, if it exists;
- 5 find a cycle, if it exists.

Depth-First Search: Algorithm

- Recursive algorithm: starting from vertex s, visits all the vertices in the connected component of C_s of s and labeling all edges of C_s
- Every vertex $v \in V$ has a field v.ID, with v.ID = 1 if v has been visited, and v.ID = 0 otherwise.
- Every edges e ∈ E has a filed e.label with e.label = null if e
 has not been labeled, and one between the labels DISCOVERY EDGE
 or BACK EDGE otherwise.
- During the execution of the algorithm, we say that a vertex u is
 discoverable from v if there exists a path from u to v made of
 vertices not already visited.

Depth-First Search: Algorithm

```
Algorithm DFS(G, v) (first call: v = s)
Input: undirected graph G = (V, E), vertex v \in V not visited
Output: all vertices discoverable from v visited, and all edges
         incident to them labeled as DISCOVERY or BACK EDGE
visit v; v.ID \leftarrow 1;
forall e \in G.incidentEdges(v) do
   if (e.label = null) then
       w \leftarrow G.opposite(v, e);
      if (w.ID = 0) then
      e.label \leftarrow DISCOVERY EDGE;
       DFS(G, w);
       else e.label ← BACK EDGE;
return;
```

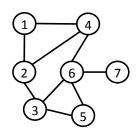
Assumptions for Implementation

- incidentEdges(v) returns an iterators on the neighbours of v (i.e., on the elements of the adjacency list of v), and the **forall** loop access them iteratively, in time Θ (1) for each of them
- opposite (v, e) returns the vertex of e opposite to v, in time $\Theta(1)$
- when the first call DFS(G,s) is made, all vertices are not visited (v.ID= 0 for all v ∈ V), and all edges are not labeled (e.label=null for all e ∈ E)

Note: for a generic call DFS(G, v) some vertices of the connected component of v may be already visited and some edges may be already labeled.

Example

Example







Adjacency lists

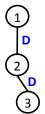
1: 2 4 2: 1 3 4

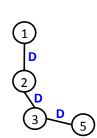
3: 2 5 6 4: 1 2 6

4: 1 2 6

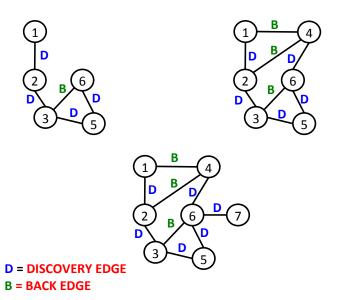
6. 2 4 5

7: 6





Example (continue)



Analysis of DFS(G,s)

- G = (V, E) undirected graph, $s \in V$
- $C_s \subseteq G$: connected component of G containing S.

Proposition

Assume to execute DFS(G,s) and that, at the beginning, the vertices and edges of C_s are not visited and not labeled. At the end of the execution:

- all the vertices of C_s are visited and all the edges of C_s are labeled as DISCOVERY o BACK EDGE;
- 2 the DISCOVERY EDGES are a spanning tree T of C_s rooted in s.

Proof: see the material online.

Complexity of DFS(G, s)

Theorem

Assume to execute DFS(G,s) and that, at the beginning, the vertices and edges of C_s are not visited and not labeled. The complexity of DFS(G,s) is Θ (m_s), where m_s is the number of edges of C_s .

Note: if G = (V, E) is connected, the complexity of DFS(G, s) is $\Theta(|E|)$.

Similarly to what we have seen for the BFS, the following result is easy to prove.

Proposition

Given G = (V, E), with |V| = n and |E| = m, the following problems can be solved in time O(m + n) using the DFS:

- 1 test if G is connected;
- 2 find the connected components of G;
- 3 find a spanning tree of G, if G is connected:
- 4 find a path between s and t, if it exists (s-t reachability);
- 5 find a cycle, if it exists.