Lecture 24
Search in Graphs

15-122: Principles of Imperative Computation (Spring 2019)
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In this lecture, we will discuss the question of *graph reachability*: given two vertices v and w, does there exist a path from v to w?

This maps as follows onto the learning goals for this course:

Computational Thinking: We continue learning about graphs, and specifically about paths in a graph. An important question is whether there exists a path between two given nodes. A related problem is to produce this path (if it exists).

Algorithms and Data Structures: We explore two classic approaches to answering these questions: depth-first search and breadth-first search. Both rely on the need to remember what we have done already, and to go back and try something else if we get stuck.

Programming: We give two implementations of depth-first search, one recursive that uses the call stack of C to remember what we have done, and the other iterative that uses an explicit stack for that purpose. We also see that breadth-first search is the variant of the latter where a queue is used instead of a stack.

As a reminder, we are working with the following minimal graph interface. We will be implementing our search in terms of this interface.

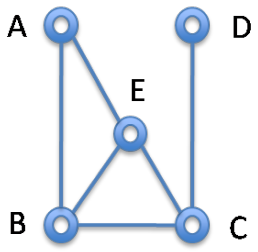
```
typedef unsigned int vertex;
typedef struct graph_header *graph_t;

graph_t graph_new(unsigned int numvert);
//@ensures \result != NULL;

void graph_free(graph_t G);
//@requires G != NULL;

unsigned int graph_size(graph_t G);
//@requires G != NULL;

bool graph_hasedge(graph_t G, vertex v, vertex w);
//@requires G != NULL;
//@requires v < graph_size(G) && w < graph_size(G);

void graph_addedge(graph_t G, vertex v, vertex w);
//@requires G != NULL;
//@requires v < graph_size(G) && w < graph_size(G);
//@requires v != w && !graph_hasedge(G, v, w);

typedef struct vert_list_node vert_list;
struct vert_list_node {
  vertex vert;
  vert_list *next;
};

vert_list* graph_get_neighbors(graph_t G, vertex v);
//@requires G != NULL;
//@requires v < graph_size(G);

void graph_free_neighbors(vert_list* neighbors);
```

1 Paths in Graphs

A *path* in a graph is a sequence of vertices where each vertex is connected to the next by an edge. That is, a path is a sequence

$$v_0, v_1, v_2, v_3, \ldots, v_l$$

of some length $l \geq 0$ such that there is an edge from v_i to v_{i+1} in the graph for each $i < l$.



For example, all of the following are paths in the graph above:

$$A - B - E - C - D$$
$$A - B - A$$
$$E - C - D - C - B$$
$$B$$

The last one is a special case: The length of a path is given by the number of edges in it, so a node by itself is a path of length 0 (without following any edges). Paths always have a starting vertex and an ending vertex, which coincide in a path of length 0. We also say that a path connects its endpoints.

The *graph reachability problem* is to determine if there is a path connecting two given vertices in a graph. If we know the graph is connected, this problem is easy since one can reach any node from any other node. But we might refine our specification to request that the algorithm return not just a boolean value (reachable or not), but an actual path. At that point the problem is somewhat interesting even for connected graphs. In complexity theory it is sometimes said that a path from vertex v to vertex w is a *certificate* or *explicit evidence* for the fact that vertex w is reachable from another vertex v. It is easy to check whether the certificate is valid, since it is easy to check if each node in the path is connected to the next one by an edge. It is more difficult to produce such a certificate.

For example, the path

$$A - B - E - C - D$$

is a certificate for the fact that vertex D is reachable from vertex A in the above graph. It is easy to check this certificate by following along the path and checking whether the indicated edges are in the graph.

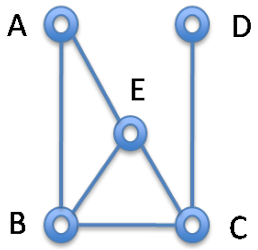
In most of what follows we are not concerned with finding the path, but only with determining whether one exists. It is not difficult to see how to extend the algorithms we discuss to compute the path as well.

2 Depth-First Search

The first algorithm we consider for determining if one vertex is reachable from another is called *depth-first search*.

Let's try to work our way up to this algorithm. Assume we are trying to find a path from u to w. We start at u. If it is equal to w we are done, because w is reachable by a path of length 0. If not we pick an arbitrary edge leaving u to get us to some node v. Now we have "reduced" the original problem to the one of finding a path from v to w.

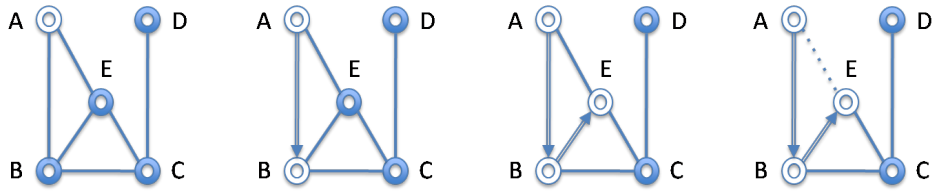
The problem here is of course that we may never arrive at w even if there is a path. For example, say we want to find a path from A to D in our earlier example graph.



We can go $A - B - E - A - B - E - \cdots$ without ever reaching D (or we can go just $A - B - A - B - \cdots$), even though there exists a path.

We need to avoid repeating nodes in the path we are exploring. A *cycle* is a path of length 1 or greater that has the same starting and ending point. So another way to say we need to avoid repeating nodes is to say that we need to avoid cycles in the path. We accomplish this by *marking* the nodes we have already considered so when we see them again we know not to consider them again.

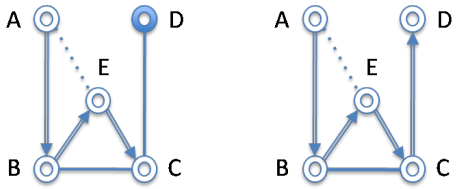
Let's go back to the earlier example and play through this idea while trying to find a path from A to D. We start by marking A (indicated by hollowing the circle) and go to B. We indicate the path we have been following by drawing a double-line along the edges contained in it.



When we are at B we mark B and have three choices for the next step.

1. We could go back to A, but A is already marked and therefore ruled out.
2. We could go to E.
3. We could go to C.

Say we pick E. At this point we have again three choices. We might consider A as a next node on the path, but it is ruled out because A has already been marked. We show this by dashing the edge from A to E to indicate it was considered, but ineligible. The only possibility now is to go to C, because we have been at B as well (we just came from B).

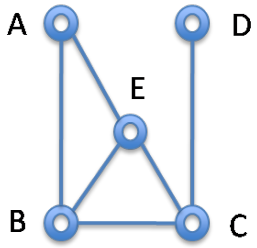


From C we consider the link to D (before considering the link to B) and we arrive at D, declaring success with the path

$$A - B - E - C - D$$

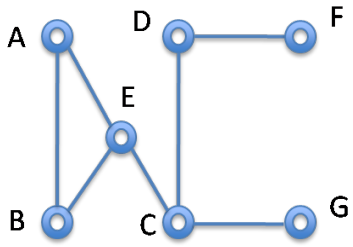
which, by construction, has no cycles.

There is one more consideration to make, namely what we do when we get stuck. Let's reconsider the original graph



and the goal to find a path from E to B. Let's say we start $E - C$ and then $C - D$. At this point, all the vertices we could go to (which is only C) have already been marked! So we have to *backtrack* to the most recent choice point and pursue alternatives. In this case, this could be C, where the only remaining alternative would be B, completing the path $E - C - B$. Notice that when backtracking we have to go back to C even though it is already marked.

Depth-first search is characterized not only by the marking, but also that when we get stuck we always return to our most recent choice and follow a different path. When no other alternatives are available, we backtrack further. Let's consider the following slightly larger graph, where we explore the outgoing edges using the alphabetically last label first. We will trace the search for a path from A to B.



We write the current node we are visiting on the left and on the right a *stack* of nodes we have to return to when we backtrack. For each of these we also remember which choices remain (in parentheses). We annotate marked nodes with an asterisk, which means that we never pick them as the next node to visit.

For example, going from step 4 to step 5 we do not consider E^* but go to D instead. We backtrack when no unmarked neighbors remain for the current node. We are keeping the visited nodes on a stack so we can easily return to the most recent one. The stack elements are separated by | and

the lists of neighbors are wrapped in parentheses, e.g., (B, A^*).

Step	Current	Stack	*Remark*
1	A		
2	E	$A^*\ (B)$	
3	C	$E^*\ (B, A^*) \mid A^*\ (B)$	
4	G	$C^*\ (E^*, D) \mid E^*\ (B, A^*) \mid A^*\ (B)$	*Backtrack*
5	D	$C^*\ () \mid E^*\ (B, A^*) \mid A^*\ (B)$	
6	F	$D^*\ (C^*) \mid C^*\ () \mid E^*\ (B, A^*) \mid A^*\ (B)$	*Backtrack*
7	B	$E^*\ (A^*) \mid A^*\ (B)$	*Goal Reached*

2.1 Recursive Depth-First Search

Now we can easily write the depth-first search code recursively, letting the *call stack* keep track of everything we need for backtracking.

```
1  bool dfs_helper(graph_t G, bool *mark, vertex start, vertex target) {
2    REQUIRES(G != NULL && mark != NULL);
3    REQUIRES(start < graph_size(G) && target < graph_size(G));
4    REQUIRES(!mark[start]);
5
6    // mark start as seen
7    mark[start] = true;
8
9    // there is an edge from start to v and a path from v to target if...
10   // target == start, or
11   if (target == start) return true;
12   // there is an edge from start to v ...
13   vert_list *nbors = graph_get_neighbors(G, start);
14   for (vert_list *p = nbors; p != NULL; p = p->next) {
15     vertex v = p->vert;   // v is one of start's neighbors
16     // ... and a path from v to target
17     if (!mark[v] && dfs_helper(G, mark, v, target)) {
18       graph_free_neighbors(nbors);
19       return true;
20     }
21   }
22   graph_free_neighbors(nbors);
23   return false;
24 }
```

We shall free the neighbor list before each return, or risk a memory leak.

We've named the function `dfs_helper` because the user of the search should not have to worry about supplying the array of marks. Instead the user calls the function `dfs`, below, which creates the marks and passes them to the recursive helper function.

```
26 bool dfs(graph_t G, vertex start, vertex target) {
27   REQUIRES(G != NULL);
28   REQUIRES(start < graph_size(G) && target < graph_size(G));
29
30   bool *mark = xcalloc(graph_size(G), sizeof(bool));
31   bool connected = dfs_helper(G, mark, start, target);
32   free(mark);
33   return connected;
34 }
```

What is the cost of recursive DFS for a graph with v vertices and e edges?

The function `dfs` creates an array of marks with all positions initialized to zero (i.e., to `false`) on line 30. Although this array has v elements, the operating system, which ultimately appropriates the blocks of memory handed out by `malloc` and `calloc`, is able to perform this operation in about $O(1)$ time. The call to `free` is also constant time. Therefore, the asymptotic complexity of `dfs` is equal to the cost of the call to `dfs_helper` on line 31.

The analysis of `dfs_helper` bears similarities to that of `graph_print` in the last chapter, with the novelty that `dfs_helper` is recursive rather than iterative. The call to `graph_get_neighbors` on line 13 has constant cost in the adjacency list representation and costs $O(v)$ in the adjacency matrix representation. The body of the loop on lines 14–21 runs $O(e)$ times *overall* since every edge will be visited exactly twice altogether (once from each direction). In particular, line 15 is run $O(e)$ times altogether.

This entails that there will be at most $2e$ recursive calls to `dfs_helper`. Furthermore, lines 4 and 7, and the fact that marks are never reset, ensures that this function will be called no more than v times. Thus, there can be at most $\min(2e, v)$ recursive calls to `dfs_helper`.

Each call to `graph_free_neighbors` costs $O(1)$ in the adjacency list representation while they altogether cost $O(e)$ in the adjacency matrix representation. All other operations in `dfs_helper` have constant cost, and therefore $O(\min(e, v))$ overall since there are at most $\min(2e, v)$ recursive calls.

Tallying up all these components, we have an $O(e)$ worst case complexity for the call to `dfs_helper` on line 31 with an adjacency list representation and $O(\min(v^2, ev))$ for the adjacency matrix representation — the latter is often simplified to $O(v^2)$ since most graphs encountered in realistic applications have at least $O(v)$ edges. This is also the cost of `dfs`.

2.2 Depth-First Search with an explicit stack

When scrutinizing the above example, we notice that the sophisticated data structure of a stack of nodes with their adjacency lists was really quite unnecessary for DFS. The recursive implementation is simple and elegant, but its effect is to make the data management more complex than necessary: all we really need for backtracking is a stack of nodes that have been seen but not yet considered.

This can all be simplified by making the stack explicit. In that case there is a single stack with all the nodes on it that we still need to look at. (In the sample code in Figure 1, we use a stack specialized to hold things of type `vertex` just to keep the code simple.)

Step	Current	Neighbors	New stack
0			(A^*)
1	A^*	(E, B)	(E^*, B^*)
2	E^*	(C, B^*, A^*)	(C^*, B^*)
3	C^*	(G, E^*, D)	(G^*, D^*, B^*)
4	G^*	(C^*)	(D^*, B^*)
5	D^*	(F, C^*)	(F^*, B^*)
6	F^*	(D^*)	(B^*)
7	B^*	(E^*, A^*)	$()$

In the code in Figure 1, we mark the starting node and push it on the stack. Then we iteratively pop the stack and examine each neighbor of the node we popped. If the neighbor is not already marked, we push it on the stack to make sure we look at it eventually. If the stack is empty then we've explored all possibilities without finding the target, so we return `false`.

While convincing, this explanation comes short of a proof that our implementation is correct, i.e., that it returns `true` when there is a path between `start` and `target` and returns `false` otherwise. We will now develop a more solid argument, although we will stop short of a formal proof. The function `dfs_explict_stack` returns in exactly three places. The first is on line 5, when `start` is equal to `target`. By definition, there is a degenerate path between these two nodes in this case.

```c
bool dfs_explicit_stack(graph_t G, vertex start, vertex target) {
  REQUIRES(G != NULL);
  REQUIRES(start < graph_size(G) && target < graph_size(G));

  if (start == target) return true;

  // mark is an array containing only the start
  bool *mark = xcalloc(graph_size(G), sizeof(bool));
  mark[start] = true;

  // Work list initially containing only start
  istack_t S = stack_new();
  push(S, start);

  while (!stack_empty(S)) {
  // Loop invariants to prove correctness go here
    vertex v = pop(S);      // v is the current node
    vert_list *nbors = graph_get_neighbors(G, v);
    for (vert_list *p = nbors; p != NULL; p = p->next) {
      vertex w = p->vert;  // w is one of v's neighbors
      if (w == target) {   // if w is the target return true
        graph_free_neighbors(nbors);
        stack_free(S);
        free(mark);
        return true;       // Success!
      }
      if (!mark[w]) {      // if w was not seen before
        mark[w] = true;       // Mark it as known
        push(S, w);           // Add to work list
      }
    }
    graph_free_neighbors(nbors);
  }
  stack_free(S);
  free(mark);
  return false;
}
```

Figure 1: Depth-first Search with an Explicit Stack

The other two places where the function returns, lines 25 and 36, have us go through loops. To reason about loops, we need to develop loop invariants that we will squeeze in the placeholder on line 16. We start with the return statement on line 25: we know that `w` (which is equal to `target` by line 21) is a neighbor of vertex `v`, but how do we know that there is a path from `start` to `v`? Two invariants will prove helpful here:

1. *Every marked vertex (i.e., a vertex `u` such that `mark[u] == true`) is connected to `start`.*

2. *Every vertex in the stack is marked.*

These two invariants hold initially since `start` is the only marked vertex and the only item in the stack before the loop is run the first time. They are preserved by an arbitrary iteration of the loop since only neighbors of `v` (which is assumed to be reachable from `start`) are marked on line 28 and they are immediately pushed on the stack on line 29. Therefore, if the loop exits at line 25, we know that there is a path from `start` to `target`.

These two invariants are not sufficient to prove that there is no path from `start` to `target` if the function returns `false` on line 36. For this, we need a new concept and a new invariant involving it. The new concept is that of *frontier* of the search. The frontier is a set of vertices that we know are connected to `start` but that we have not explored yet. At any point in the loop on lines 15–33, the frontier is the contents of the stack. The new invariant is the following:

3 *Every path from `start` to `target` passes through a vertex in the frontier.*

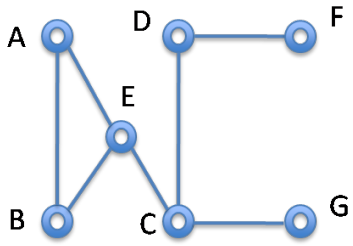
It is clearly true initially when the stack (the frontier) only contains `start`. It is preserved by the loop because intuitively a frontier element is replaced by all of its neighbors that have not been explored already. More interesting is why this invariant allows us to prove that there is no path to `target` if the function returns on line 36: for this to happen, we must have exited the loop in lines 15–33, which entails that the negation of its loop guard is true: the stack (our frontier) is empty. By our third invariant (which still holds at this point), every path from `start` to `target` must go through a vertex in the frontier. But the frontier is empty, so it contains no vertex through which such a pass can go: thus, there cannot be any path from `start` to `target`. Only in this way can the invariant be true, if the frontier is empty: if all of zero paths from `start` to `target` pass through one of the (zero) vertices in the empty frontier.

The complexity considerations we developed for the recursive version of DFS apply here as well — possibly more explicitly. The above code has cost $O(e)$ with an adjacency list representation: initializing the array of marks has cost $O(1)$, and the body of the inner loop will run $O(e)$ times, twice for each edge. The cost is $O(\min(v^2, ev))$ — just $O(v^2)$ in most situations — with an adjacency matrix representation as we have to account for the $O(v)$ cost of `graph_get_neighbors`.

3 Breadth-First Search

The iterative DFS algorithm managed its agenda, i.e., the list of nodes it still had to look at, using a stack. But there's no reason to insist on a stack for that purpose. What happens if we replace the stack by a queue? All of a sudden, we will no longer explore the most recently found neighbor first as in depth-first search, but, instead, we will look at the oldest neighbor first. This corresponds to a *breadth-first search* (BFS) where you explore the graph layer by layer. So BFS completes a layer of the graph before proceeding to the next layer. The code for that and many other interesting variations of graph search can be found on the course web page.

Here's an illustration using our running example of search for a path from A to B in the graph



Step	Current	Neighbors	New queue
0			(A^*)
1	A^*	(E, B)	(E^*, B^*)
2	E^*	(B^*, A^*, C)	(B^*, C^*)
3	B^*	(E^*, A^*)	(C^*)

We find the path much faster this way. But this is just one example. Try to think of another search in the same graph that would cause breadth-first search to examine more nodes than depth-first search would.

The code looks the same as our iterative depth-first search, except for the use of a queue instead of a stack. Therefore we do not include it here.

You could write it yourself, and if you have difficulty, you can find it in the code folder that goes with this lecture. Note that our correctness and complexity analysis for DFS never relied on using a stack. Thus, it remains sound once we swap the stack for a queue. Correctness also hold for any other implementation of work list, but complexity may need to be revisited if these implementation cannot provide constant-time insertion and retrieval operations.

4 Conclusion

Breadth-first and depth-first search are the basis for many interesting algorithms as well as search techniques for artificial intelligence.

One potentially important observation about breadth-first versus depth-first search concerns search when the graph remains implicit, for instance in game search. In this case there might be infinite paths in the graph. Once embarked on such a path depth-first search will never backtrack, but will pursue the path endlessly. Breadth-first search, on the other hand, since it searches layer by layer, is not subject to this weakness (every node in a graph is limited to a finite number of neighbors). In order to get some benefits of both techniques, a technique called *iterative deepening* is sometimes used.