Depth First Search

A

4

3

2

4

B

3

5

4

2

C

4

5

4

3

D

5

E

3

4

2

F

2

3

G

3

2

2

3
The idea of DFS (Depth-First Search) is to explore the graph by always taking a step from the most recently seen vertex – when we can’t go to a new vertex, we back up and go forward from the most recent vertex that still has any unvisited neighbours.

Using the graph shown above, if we start at vertex E the candidates for the next vertex are E’s neighbours G, A and F – we choose one of them - this choice is random or arbitrary – suppose we choose A. From A, the unvisited neighbours are D and B. Suppose we choose D. D’s unvisited neighbours are B and G … and so on.

The DFS algorithm is very simple to express:

```python
def DFS(v):
    mark v “visited”
    for each neighbour y of v:
        if y is not visited:
            DFS(y)
```

This expression of the algorithm gains elegance by using recursion to manage all the “back up and go forward” operations. Unfortunately, we know that recursive algorithms involve more overhead and are often slower in execution than iterative versions of the same algorithm.

As with many recursive algorithms we can replace the recursion in DFS with a loop, just by implementing a stack.

Note: there was an error in the version of this algorithm that I showed in class on Monday. The following is correct:
def DFS(v):
    create a stack S
    S.push(v)
    while not S.isEmpty():
        x = S.pop()
        if x is not visited:
            for each neighbour y of x:
                if y is not visited:
                    S.push(y)
            mark x "visited"

The error in the version shown in class was in marking the vertices as “visited” too early. Basically, in DFS we need to mark vertices when they come off the stack, not when they go on it.

You should confirm that this executes a proper Depth-First Search of a graph.

If you compare the BFS and DFS algorithms you will see that the only significant difference between them is the data structure – a queue for BFS and a stack for DFS. Since the basic operations on queues and stacks are all in O(1), this means that the over-all complexity is exactly the same for the two algorithms. This is a great illustration of the idea that knowing the properties of data structures can greatly simplify the analysis of algorithms.

It’s also a great illustration of the power of choosing the right data structure – it’s kind of magical that by changing the queue to a stack, the algorithm changes from doing a breadth-first search to a depth-first search.

We should note that both BFS and DFS can be used to determine if a graph is connected. BFS is also useful because (as we know) in an unweighted graph it finds the shortest paths from the start vertex to all other vertices. It would be really nice if we could claim that DFS finds the longest paths from the start vertex to all other vertices … well we could claim that, but we would be wrong. DFS cannot guarantee that it will find either shortest or longest paths.

It turns out that DFS is the perfect graph-searching method for some really interesting problems … but they are outside the scope of this course. You will just have to live in suspense for a bit longer!
Minimum (Weight) Spanning Trees

Let G be a graph with weights on the edges. We define the **weight** of any subgraph of G to be the sum of the weights of the edges in the subgraph.

One of the classic problems in graph theory can be stated thusly: given a connected graph G with non-negative weights on the edges, find a subgraph T of G such that:

1. T contains all vertices of G
2. T is connected
3. the weight of T is \( \leq \) the weight of every subgraph that satisfies requirements 1 and 2

It is not hard to see that T must be a tree – if T contains a cycle we can reduce its weight by eliminating one edge of the cycle. This explains the choice of “T” as the name of the subgraph we are looking for.

So our goal here is to find a minimum weight spanning tree … and because humans love shortcuts, we always leave out the word “weight” and just call this the Minimum Spanning Tree problem … which we abbreviate even further to “the MST problem”.

We have already seen two algorithms that find spanning trees of a graph: Breadth-First Search and Depth-First Search. These both ignore weights on the edges and so they obviously can’t be counted on to find a minimum spanning tree … but it might seem plausible that we could somehow modify them to solve this problem.

For example, in BFS we add neighbours of the current vertex to the queue in a random order … what if we added them in order of the weight of the edges that join them to the current vertex? Similarly, in DFS we might decide to always choose the neighbour of the current vertex that has the lowest-weight edge from the current vertex. Try to find graphs where these modifications fail to find a MST.

Those suggestions may have got you thinking about some of the other data structures we have studied. For example, is there some way that BFS or DFS could put vertices into a priority queue so that we choose the next vertex in such a way that we do get a MST? Well … hold that thought!

There are many algorithms that solve the MST problem – we will look at two of the most famous ones. We’ll spend a lot more time on the first one because once you understand that, the other is very easy to learn.
Prim’s Algorithm

The algorithm that we are calling Prim’s Algorithm was actually first discovered in 1930 by Jarnik. Prim rediscovered it in 1957, and Dijkstra re-discovered it in 1959. Because of this history it is sometimes called Jarnik’s Algorithm, the Prim-Jarnik Algorithm, the Prim-Dijkstra Algorithm, or the DJP Algorithm. I’ll stick with Prim’s Algorithm.

Prim’s Algorithm effectively grows a MST from scratch: it starts with a single vertex, then chooses an edge that connects another vertex to the first one, then chooses another edge that connects another vertex to one of the two already chosen, and so on. The tree continues to grow until it contains all n vertices. The criterion by which edges are selected is really simple: we always choose the least-weight edge that has one end in the tree and one end in the set of vertices we haven’t reached yet.

You may be asking questions like:
- Dr. Prim, how do we decide which vertex to start at?
- What do we do if two or more edges are tied for being the least-weight edge from the tree to the rest of the graph?

Here’s the tough-guy answer that Prim gives to both of these questions:
- It doesn’t matter which one you pick. I’ll still find a MST. You can’t stop me. Mwah-hah-ha-ha!

We’ll prove that Prim’s Algorithm always finds the right answer in the next installment of these notes. First we need to express the algorithm in a semi-formal way, and talk about its implementation.

def Prim(G):
    # G is a connected graph with weighted edges
    choose any vertex v
    chosen_edges = {}
    T = {v}  # T is the tree we are growing
    R = {all vertices except v}  # R is the rest of the vertices
    while |T| < n:
        # keep going until T contains all vertices
        let e be the least-weight edge that has one end in T
        and one end in R
        suppose e = (x,y) with x in T and y in R
        add e to chosen_edges
        add y to T
        remove y from R
Everything in that algorithm is trivial except for

\[
\text{let } e \text{ be the least-weight edge that has one end in } T \text{ and one end in } R
\]

We need to think very carefully about how to implement the location and selection of the appropriate edge.

There are at least four solutions.

**Solution 1:**

We can take the set of all edges and sort them into ascending-weight order. This takes \(O(m \log m)\) time. Now when we choose the least-weight edge that has one end in \(T\) and one end in \(R\), we can do that by searching the list of edges from the beginning and stopping as soon as we find an edge that meets the criterion. Note that every search has to start at the beginning of the list because the low-weight edges may have had both ends in \(R\). So we have to do \(n-1\) searches (to choose the \(n-1\) edges of the MST) and each search takes \(O(m)\) time ... this gives \(O(m \times n)\) as the complexity. That’s pretty bad ... let’s try again.

**Solution 2:**

At each iteration we need an edge that has the smallest weight, out of the edges that are available (ie that have one end in \(T\) and the other end in \(R\)). We have seen a data structure that makes it easy to repeatedly find the largest element, but here we need to find the smallest element. So instead of a Max-heap, we need a Min-heap. Fortunately the structural rules of Min-heaps are identical to Max-heaps, and the “relational” rule is just reversed: each value is \(\leq\) its children, rather than \(\geq\) its children. This results in the smallest item being at the root.

We could start by putting all the edges into the heap, but this would be wasteful – the edge at the top of the heap might not be usable because both of its ends are in \(R\) – we would need to remove it and then re-insert it into the heap later. To avoid this, we only add edges to the heap when they have one end in \(T\) and one end in \(R\). Later we may need to discard some of these edges because both ends are now in \(T\), but that’s not too much trouble.

We can write this version of Prim’s MST Algorithm quite completely. This assumes that there is a function \(weight(x,y)\) that returns the weight of the edge joining \(x\) and \(y\).
def Prim(G):    # G is a connected graph with weighted edges
    choose any vertex v
    chosen_edges = {}
    T = {v}    # T is the tree we are growing
    R = {all vertices except v}    # R is the rest of the vertices
    create a Min-heap called M
    for each neighbour y of v:
        add the item [(v,y), weight(v,y)] to M, using the
        weight value as the “priority”
    while |T| < n:    # keep going until T contains all
        # vertices
        e = M.remove_top()
        # e consists of a pair of vertices (a,b) and a weight value
        # When e was added to the Min-heap, a was in T and b was in
        # R ... we need to see if that is still true ... if not we need
        # to try the new top item in M
        while b in T:    # loop until we have a usable edge
            e = M.remove_top()
            # e = (a,b) with a in T and b in R
            add e to chosen_edges
            add b to T
            remove b from R
            for each neighbour y of b:
                if y in R:
                    add the item [(y,b), weight(y,b)] to M, using
                    the weight value as the “priority”
    return chosen_edges

Now we can work out the complexity of this version of the algorithm. Clearly the
“remove_top” operations are the dominant steps. In the worst case, every edge will
eventually be added to the heap, and every edge will eventually be removed from the heap.
Since the maximum size of the heap is m, we know adding to the heap and removing the top element from the heap are both in O(log m). Combining this with the statement that each of
these steps could execute m times, we end up with m * O(log m) which is equal to O(m * log
m)

But we can simplify that a bit – recall that m < \frac{n^2}{2}

so log(m) < \log \left( \frac{n^2}{2} \right) = \log(n^2) - \log 2 = 2\log(n) - 1, which is in O(log n)

This means we can rewrite O(m * log m) as O(m * log n) ... which is a lot better than O(m*n)
Clearly if the graph is sparse, with \( m \) in \( O(n) \), then this algorithm runs in \( O(n \times \log n) \) time.

However if the graph is dense, with \( m \) in \( \Omega(n^2) \), then this algorithm runs in \( O(n^2 \times \log n) \) time.

Maybe we can beat that … we have two more possible solutions to look at.

**Solution 3:**

In Solution 2 we spent a lot of time putting edges in and out of a big Min-heap, and there was always a possibility that we would have to remove many edges from the top of the heap before finding one we could use. We can attempt to avoid this by using a heap containing vertices instead of edges.

In this solution, we use a heap that contains one node for each vertex in \( R \). Every time we add a vertex to \( T \), we see if it gives us a new, less costly connection to any of the vertices in \( R \). If it does, we move the corresponding node upwards in the heap (ohhhhh, this is why we learned about changing priorities of items in a heap!)

This heap will initially contain \( n-1 \) nodes (the start vertex never needs to be in the heap). The node at the top will correspond to the vertex in \( R \) with the least cost edge to \( T \), so we know we can always use the top node – there will never be a need to discard the top node and get another one.

This is looking good … let’s look at it closely. There are no insert operations since we build the heap with all \( n-1 \) vertices of \( R \), and after that we only remove things. Each remove_top operation takes \( O(\log n) \) time and there are only \( n-1 \) vertices to remove, so it looks like we are heading towards \( O(n \times \log n) \) complexity. But … we also have to consider the updates.

Doing an individual update on the heap takes \( O(\log n) \) time … so if we do the updates individually, the total amount of work spent on heap updates is \( O(m \times \log n) \) because each edge might cause an update. This means that for sparse graphs the algorithm is in \( O(n \times \log n) \). However, if the graph is very dense (complete or nearly complete) then it is possible that every time we add a vertex to \( T \), it *could* give us a reduced cost to *every* vertex in \( R \). Doing the heap updates individually will be \( O(n^2 \times \log n) \). This is just the same as Solution 2.

However, we know from our study of heaps that if we need to update the priority of every item in the heap, the best thing to do is just rebuild the heap from scratch – and that is an \( O(n) \)
operation. If we rebuild the heap on each iteration of the loop, we end up with $O(n^2)$ for the whole algorithm. This is better than Solution 2 for dense graphs, but worse on sparse graphs.

The problem with this version of the algorithm is deciding when we should rebuild the heap, and when we should just do the updates one by one. One option would be to rebuild the heap whenever the number of updates caused by a single vertex is greater than some threshold value, but do the updates one at a time when the number is below this threshold. Determining an appropriate threshold value is a very difficult problem – it helps if you have a priori knowledge about the size and density of the graphs you will be dealing with. If you do have this information you can simply have two versions of the algorithm – one for sparse graphs and one for dense graphs.

This difficulty comes from the fact that for a specific graph $G$ with $n$ vertices and $m$ edges, we can certainly say that $G$ is sparse if $m$ is close to $n$, and $G$ is dense if $m$ is close to $\binom{n}{2}$... but values of $m$ that are near the middle of the range of possibilities are harder to classify.

You can work out the pseudo-code for this version of Prim’s Algorithm – it is a lot like Solution 2, with added operations to do the heap updates/rebuilds.

**Solution 4:**

We can simplify Solution 3 by ditching the heap (oh no, I liked the heap). We can just keep an array of all the vertices in $R$, together with their minimum cost to connect to $T$, and the vertex they would connect to (this allows us to keep track of the edges we are using). Every time we add a vertex to $T$, we look at its neighbours and, if necessary, we update their “best connection” info. To find the next vertex to connect, we just do a linear search of the array. This array would look something like this (I have added row labels)

<table>
<thead>
<tr>
<th>Vertex</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>...</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>Still in R?</td>
<td>N</td>
<td>N</td>
<td>Y</td>
<td>Y</td>
<td>...</td>
<td>Y</td>
</tr>
<tr>
<td>Connector</td>
<td>-</td>
<td>-</td>
<td>2</td>
<td>12</td>
<td>...</td>
<td>6</td>
</tr>
<tr>
<td>Cost</td>
<td>-</td>
<td>-</td>
<td>8</td>
<td>3</td>
<td>...</td>
<td>9</td>
</tr>
</tbody>
</table>

Suppose that on the next iteration we find that vertex 4 has the lowest connection cost. We add the edge (12,4) to our set of Tree edges, we add vertex 4 to $T$, and we update vertex 4’s neighbours. Suppose there is an edge from vertex 4 to vertex n with cost 7. This is an
improvement over the current cost (9) to connect vertex n, so we update this information. Suppose there is an edge from vertex 4 to vertex 2 – we ignore this because vertex 2 is not in R – it has already been added to T. Suppose there is an edge from vertex 4 to vertex 3 with cost 15. This is greater than the current cost to connect to vertex 3, so we ignore it.

The array would now look like this:

<table>
<thead>
<tr>
<th>Vertex</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>...</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>Still in R?</td>
<td>N</td>
<td>N</td>
<td>Y</td>
<td>N</td>
<td>...</td>
<td>Y</td>
</tr>
<tr>
<td>Connector</td>
<td>-</td>
<td>-</td>
<td>2</td>
<td>-</td>
<td>...</td>
<td>4</td>
</tr>
<tr>
<td>Cost</td>
<td>-</td>
<td>-</td>
<td>8</td>
<td>-</td>
<td>...</td>
<td>7</td>
</tr>
</tbody>
</table>

We would start the next iteration by searching the array for the vertex in R with the lowest connection cost, and repeat the update process.

The complexity of this version of Prim’s Algorithm is very easy to determine. We need n-1 iterations, each of which involves a linear search of the array – this is $O(n^2)$. The total number of updates is $\leq m$, and each update takes constant time. Thus the entire algorithm takes $O(n^2 + m)$ time … but since $m < n^2$, this simplifies to $O(n^2)$. Note that this version is not sensitive to the density of the graph – it is $O(n^2)$ whether the graph is sparse or dense. Pseudo-code for this algorithm looks something like this:
def Prim(G):
    # we will start our tree with vertex 1 - why not?
    Create array A with three rows (1,2,3) and n columns (1, ... n)
    # row 1 is “Still in R”
    # row 2 is the connector vertex
    # row 3 is the cost
    # note that I have not bothered with a row to store the vertex
    # numbers since they are just the column numbers
    A[1][1] = N # vertex 1 is not in R
    for x = 2 .. n:
        A[1][x] = Y
        A[2][x] = -
        A[3][x] = infinity
    for each neighbour y of vertex 1:
        A[2][y] = 1
        A[3][y] = weight(1,y)

    T = {1}
    chosen_edges = {}
    while |T| < n:
        search A for the vertex still in R with the smallest
        value in the third row
        let this vertex be x
        add x to T
        add the edge (x,A[2][x]) to chosen_edges
        A[1][x] = N
        A[2][x] = - # these are not really needed, they just
        A[3][x] = - # make it easier to see which vertices are
        # still available
        for each neighbour y of x:
            if y is still in R and weight(x,y) < A[3][y]:
                A[2][y] = x
                A[3][y] = weight(x,y)
Concluding Observations::

Solution 1 is just bad.

Solution 2 is efficient on sparse graphs, but inefficient on dense graphs.

Solution 3 can have exactly the same complexity as Solution 2 (good on sparse, not so good on dense), or exactly the same complexity as Solution 4 (good on dense, not so good on sparse). It is difficult to achieve the best of both worlds.

Solution 4 has the same complexity on all graphs (which makes it good for dense graphs, but not so good for sparse graphs).

<table>
<thead>
<tr>
<th></th>
<th>Sparse Graphs</th>
<th>Dense Graphs</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( m \in O(n) )</td>
<td>( m \in \Omega(n^2) )</td>
</tr>
<tr>
<td>Solution 1</td>
<td>( O(n^3) )</td>
<td>( O(n^3) )</td>
</tr>
<tr>
<td>Solution 2</td>
<td>( O(n \cdot \log n) )</td>
<td>( O(n^2 \cdot \log n) )</td>
</tr>
<tr>
<td>Solution 3</td>
<td>( O(n \cdot \log n) ) or ( O(n^2) )</td>
<td>( O(n^2 \cdot \log n) ) or ( O(n^2) )</td>
</tr>
<tr>
<td>Solution 4</td>
<td>( O(n^2) )</td>
<td>( O(n^2) )</td>
</tr>
</tbody>
</table>

The complexity of Solution 3 depends on whether we do the heap updates individually or by rebuilding the heap on each iteration.

Is this the end of the Prim story? Not at all! Using data structures called Fibonacci Heaps it is possible to reduce the complexity to \( O(m + n^*\log n) \) for all graphs … and the search continues for further improvements.