Material in this lecture:
- Breadth First Search
- Unweighted Shortest Paths

1 Breadth First Search

The first graph search approach we consider is breadth first search (BFS). BFS can be applied to solve a variety of problems including: finding all the vertices reachable from a vertex \( v \), finding if an undirected graph is connected, finding the shortest path from a vertex \( v \) to all other vertices, determining if a graph is bipartite, bounding the diameter of an undirected graph, partitioning graphs, and as a subroutine for finding the maximum flow in a flow network (using Ford-Fulkerson’s algorithm). BFS, as with the other graph searches, can be applied to both directed and undirected graphs. In the directed case we only consider the outgoing arcs when searching.

The idea of breadth first search is to start at a source vertex \( s \) and explore the graph level by level, first visiting all vertices that are the (out-)neighbors of \( s \) (i.e. have distance 1 from \( s \)), then vertices that have distance two from \( s \), then distance three, etc. It should be clear that a vertex at distance \( i + 1 \) must have an (in-)neighbor from a vertex a distance \( i \). Therefore, if we know all vertices at distance \( i \), then we can find the vertices at distance \( i + 1 \) by just considering their (out-)neighbors.

As with all the search approaches, the BFS needs to keep track of which vertices have already been visited so that it does not visit them more than once. We will refer to all visited vertices at the start of step \( i \) as \( X_i \). Since on step \( i \) we visit vertices at a distance \( i \) away, the vertices in \( X_i \) are exactly those with distance less than \( i \) from the source. On each step the search also maintains a frontier. At the start of step \( i \) the frontier \( F_i \) contains all unvisited neighbors of \( X_i \), which is all vertices in the graph with distance exactly \( i \) from \( s \).

In BFS on each step we visit all vertices in the frontier. This differs from DFS which only visits one. What we do when we visit depends on the particular application of BFS, but for now we assume we simply mark the vertices as visited. This is done by simply adding the frontier to the visited vertices, i.e., \( X_{i+1} = X_i \cup F_i \). To generate the next set of frontier vertices the search simply takes the neighborhood of \( F \) and removes any vertices that have already been visited, i.e., \( F_{i+1} = N_G(F) \setminus X_{i+1} \). Recall that for a vertex \( v \), \( N_G(v) \) are the neighbors of \( v \) in the graph \( G \) (the out-neighbors for a directed graph) and for a set of vertices \( F \), that \( N_G(F) = \cup_{v \in F} N_G(v) \).

Here is pseudocode for a BFS algorithm just described. It returns the set of vertices reachable from a vertex \( s \) as well as the shortest distance to the furthest reachable vertex.

†Lecture notes by Guy E Blelloch, Margaret Reid-Miller, and Kanat Tangwongsan.
Recall that $N_G(F) = \bigcup_{v \in F} N(v)$, where $N(v)$ are the neighbors of $v$. If we are using a adjacency table representation of the graph, this can be calculated as

$$
\text{fun } N_G(F) = \text{Table.reduce Set.Union } \{\} \text{ (Table.extract}(G,F))
$$

The full SML code for the algorithm is given in the appendix at the end of these notes.

Figure 1 illustrates BFS on an undirected graph where $s$ is the central vertex. Initially, $X_0$ is empty and $F_0$ is the single source vertex $s$, as it is the only vertex that is a distance 0 from $s$. $X_1$ is all the vertices that have distance less than 1 from $s$ (just $s$), and $F_1$ contains those vertices that are on the inner concentric ring, a distance exactly 1 from $s$. The outer concentric ring contains vertices in $F_2$, which are a distance 2 from $s$. The neighbors $N_G(F_1)$ are the central vertex and those in $F_2$. Notice that some vertices in $F_1$ share the same neighbors, which is why $N_G(F)$ is defined as the union of neighbors of the vertices in $F$ to avoid duplicate vertices. In general, from which frontiers could the vertices in $N_G(F_i)$ come when the graph is undirected? What if the graph is directed? For the graph in the figure, which vertices are in $X_2$?

To prove that the algorithm is correct we need to prove the assumptions that are stated in the algorithm. In particular:

**Lemma 1.1.** In algorithm BFS when calling $BFS'(X, F, i)$, we have $X = \{v \in V_G \mid \delta_G(s, v) < i\} \land F = \{v \in V_G \mid \delta_G(s, v) = i\}$

**Proof.** This can be proved by induction on the step $i$. For the base case (the initial call) we have $X_0 = \{\}, F_0 = \{s\}$ and $i = 0$. This is true since only $s$ has distance 0 from $s$ and no vertex has distance less than 0 from $s$. For the inductive step we assume the claims are correct for $i$ and want to show it for $i + 1$. For $X_{i+1}$ we are simply taking the union of all vertices at distance less than $i$ ($X_i$) and all vertices at distance exactly $i$ ($F_i$) so this must include exactly the vertices a distance less than $i + 1$. For $F_{i+1}$ we are taking all neighbors of $F_i$ and removing the $X_{i+1}$. Since all vertices $F_i$ have distance $i$ from $s$, by assumption, then a neighbor $v$ of $F$ must have $\delta_G(s, v)$ of no more than $i + 1$. Furthermore
all vertices of distance no more than \( i + 1 \) must be reachable from a vertex at distance \( i \). Therefore the neighbors of \( F_i \) contain all vertices of distance \( i + 1 \) and only vertices of distance at most \( i + 1 \). When removing \( X_{i+1} \) we are left with all vertices of distance \( i \), as needed.

To argue that the algorithm returns all reachable vertices we note that if a vertex \( v \) is reachable from \( s \) and has distance \( d = \delta(s, v) \) then there must be another \( u \) vertex with distance \( \delta(s, u) = d - 1 \). Therefore BFS will not terminate without finding it. Furthermore, for any vertex \( v \), \( \delta(s, v) < |V| \) so the algorithm will terminate in at most \( |V| \) steps.

### 1.1 BFS extensions

So far we have specified a routine that returns the set of vertices reachable from \( s \) and the longest length of all shortest paths to these vertices. Often we would like to know more, such as the distance of each vertex from \( s \), or the shortest path from \( s \) to some vertex \( v \), i.e. the actual sequence of vertices in the path. It is easy to extend BFS for these purposes. For example the following algorithm returns a table mapping every reachable vertex \( v \) to \( \delta_G(s, v) \).

```plaintext
1 fun BFS(G, s) = let
2     fun BFS′(X, F, i) =
3         if |F| = 0 then X
4         else let
5             val X′ = X ∪ {v ↦ i : v ∈ F}
6             val F′ = N_G(F) \ domain(X′)
7             in BFS′(X′, F′, i + 1) end
8     in BFS′({}, {s}, 0) end
```

To report the actual shortest paths one can generate a shortest path tree, which can be represented as a table mapping each reachable vertex to its parent in the tree. Then one can report the shortest path to a particular vertex by following from that vertex up the tree to the root (see Figure 2). We note that to generate the pointers to parents requires that we not only find the next frontier
Figure 2: An undirected graph and two possible BFS trees with distances from $s$.

$F' = N(F)/X'$ of the frontier on each level, but that we identify for each vertex $v \in F'$ one vertex $u \in F$ such that $(u, v) \in E$. There could be multiple such edges to the vertex $v$. Indeed Figure 2 shows two possible trees that differ in what the parent is for the vertex at distance 3.

There are various ways to identify the parent. One is to post-process the result of the BFS that returns the distance. In particular for every vertex we can pick one of its (in-)neighbors with a distance one less than itself. Another way is to identify the parent when generating the neighbors of $F$. In the appendix we include sample SML code that generates the parents in this way. The ideas is that both the visited vertices $X$ and the frontier $F$ are table that maps the given vertex sets to their parent. Finding the next visited set is easy since it is just a union (or a merge on tables). Finding the next frontier requires tagging each neighbor with where it came from and then merging the results. This merge has decide how to break ties since many vertices in the frontier might have the same neighbor. In the code the first vertex is taken. See the code if you are interested, or need something like this for your homework.

To find $N_G(F)$, the code in the appendix takes the union of the sets of neighbors (one set for each $v \in F$). This time, for each $v \in F$, we generate a table $\{u \mapsto v : u \in N(v)\}$ that maps each neighbor of $v$ back to $v$. Then instead of union, we use merge to combine all these neighbor tables. In terms of our ML library this would look something like

1.2 BFS Cost

So far in the class we have mostly calculated costs using recurrences. This works well for divide-and-conquer algorithms, but, as we will see, most graph algorithms do not use divide-and-conquer. Instead for many graph algorithms we can calculate costs by counting, i.e., simply adding up the costs across a sequence of steps. Since different steps take a different amount of work,

Since BFS works in a sequence of steps, one per level, we can add up the work and span across the steps. However, the work done on each step varies since it depends on the size of the frontier on that step—in fact it depends on the number of outgoing edges from the frontier for a step. What we do know is that every reachable vertex only appears in the frontier exactly once. Therefore all their out-edges also are only processed exactly once. If we can calculate the cost per edge $W_e$ and per vertex $W_v$ for processing a frontier, then we can simply multiply these by the number of edges and vertices giving $W = W_v n + W_e m$ (recall that $n = |V|$ and $m = |E|$). For the span we can determine the
span per level $S_l$ and multiply it by the number of levels $S = S_l \cdot d$, where $d = \max_{v \in V} \delta(s, v)$ is the number of levels.

If we use the tree representations of sets and tables, we can show that the work per edge and per vertex is bounded by $O(\log n)$ and the span per step is bounded by $O(\log^2 n)$. Therefore we have:

$$W_{BFS}(n, m, d) = O(n \log n + m \log n)$$
$$= O(m \log n)$$
$$S_{BFS}(n, m, d) = O(d \log^2 n)$$

We drop the $n \log n$ term in the work since for BFS we cannot reach any more vertices than there are edges.

Now let's show that the work per vertex and edge is $O(\log n)$. We can examine the code and consider what is done on each step. In particular the only non-trivial work done on each step is the union $X' = X \cup F$, the calculation of neighbors $N = N_G(F)$ and the set difference $F' = N \setminus F$. The cost of these will depend on the size of the frontier, and in fact in the number of outedges from the frontier. We will use $||F||$ to denote the number of out edges for a frontier plus the size of the frontier, i.e., $||F|| = \sum_{v \in F} (1 + d^+_G(v))$. The costs for each step are as follows

<table>
<thead>
<tr>
<th></th>
<th>Work</th>
<th>Span</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X \cup F$</td>
<td>$O(</td>
<td></td>
</tr>
<tr>
<td>$N_G(F)$</td>
<td>$O(</td>
<td></td>
</tr>
<tr>
<td>$N \setminus F$</td>
<td>$O(</td>
<td></td>
</tr>
</tbody>
</table>

The first and last lines fall directly out of the cost spec for the set interface. The second line is a bit more involved. Recall that it is implemented as

```plaintext
fun N_G(F) = Table.reduce Set.Union {} (Table.extract(G,F))
```

The work for extract is bounded by $O(||F|| \log n)$. For the cost of the union we can use Lemma 2.1 from lecture 6. In particular merge satisfies the conditions of the Lemma, therefore the work is bound by

$$W(\text{reduce union} \{} F_{\text{ ngh}} \} = O \left( \log |F_{\text{ ngh}}| \sum_{\text{ ngh} \in F_{\text{ ngh}}} (1 + |\text{ ngh}|) \right) = O (\log n \cdot ||F||)$$

where $F_{\text{ ngh}} = \text{Table.extract}(G,F)$, and span is bounded by

$$S(\text{reduce union} \{} F_{\text{ ngh}} \} = O(\log^2 n)$$

since each union has span $O(\log n)$ and the reduction tree is bounded by $\log n$ depth.

Now we see that work per edge is $O(\log n)$ since on step $i$ we process $||F_i||$ edges and every out edge is only processed once.

Notice that span depends on $d$. In the worst case $d \in O(n)$ and BFS is sequential. As we mentioned before, many real-world graphs are shallow, and BFS for these graphs has good parallelism.
2 BFS with Single Threaded Sequences

Here we consider a version of BFS that uses sequences to represent the graph and single threaded (ST) sequences to mark the visited vertices. The advantage is that it runs in $O(m)$ total work and $O(d \log n)$ span.

We refer to a graph $G = (V, E)$ where $V = \{0, 1, \ldots, n - 1\}$ as an integer labeled (IL) graph. For an IL graph we can use the sequences to represent a graph, giving constant work access to the values stored at vertices (if using array sequences). The neighbors of each vertex can also be represented as an array sequence containing the integer indices of their neighbors. An IL graph can therefore be implemented with type:

$$(\text{int seq}) \text{ seq}.$$  

We consider the version of BFS that returns a mapping from each vertex to its parent in the BFS tree. We maintain the set of visited vertices using an $(\text{int option}) \text{ stseq}$. This allows us to update which vertices have been visited in constant work per update. In this sequence the option NONE indicates the vertex has not been visited, and SOME($v$) indicates it has been and its parent is $v$. Each time we visit a vertex, we map it to its parent in the BFS tree; the value $v$ in SOME($v$) is its parent vertex. As the updates to this sequence are potentially small compared to its length, using an stseq is efficient. On the other hand, because the set of frontier vertices is new at each level, we can represent the frontier simply as an integer sequence containing all the vertices in the frontier, allowing for duplicates.

```
1 fun BFS(G:(int seq) seq, s:int)=
2   let
3       fun BFS'(XF:int option stseq, F:int seq)=
4           if |F| = 0 then stSeq.toSeq P
5           else let
6               val N = flatten(\{(u,SOME(v)):u \in G[v] : v \in F\}) % neighbors of the frontier
7               val XF' = stSeq.inject(F, XF) % new parents added
8               val F' = \{u:(u,v) \in N | XF'[u] = v\} % remove duplicates
9               in BFS'(XF', F') end
10              val X_0 = stSeq.toSTSeq((NONE:v \in \{0,\ldots,|G| - 1\}))
11              in
12             BFS'(stSeq.update(s,SOME(s),X_0), \{s\})
13           end
```

To simplify the algorithm we change the invariant a bit. In particular on entering BFS' the sequenceXF contains parent pointers for both the visited and the frontier vertices instead of just for the visited vertices. $F$ is an integer sequence containing the frontier.

All the work is done in lines 6, 7, and 8. Also note that the stSeq.inject on line 7 is always applied to the most recent version. We can write out the following table of costs:
where \( d \) is the number of rounds (i.e. the longest path length from \( s \) to any other reachable vertex). The last two columns indicate the costs if \( XF \) was implemented as a regular array sequence instead of an stSeq. The big difference is the cost of inject. As before the total work across all rounds is calculated by noting that every out-edge is only processed in one frontier, so \( \sum_{i=0}^{d} ||F_i|| = m \).

3 SML Code

**Basic BFS.** The following SML code for BFS mirrors the pseudo-code in the notes. It uses a table that maps each vertex to a set that contains its (out-)neighbors. The function \( \text{fun } N \ G \ F \) implements \( N_G(F) \) by first using \( \text{extract} \) to get a table with only the vertices in \( F \). That is, the resulting table maps each vertex in \( F \) to its neighbors. Next, it combines all the neighbors of \( F \) into a single set. Recall that \( \text{Table.reduce } f \) combines the tables values with the function \( f \).

```sml
functor TableBFS(Table : TABLE) =
  struct
    structure Set = Table.Set
    type vertex = Table.key
    type graph = Set.set Table.table

    fun N (G : graph) (F : Set.set) =
      Table.reduce Set.union Set.empty (Table.extract (G, F))

    fun BFS_reachable (G : graph, s : vertex) =
      let
        (* Require: X = \{v in V_G | delta_G(s,v) < i\} and
         * F = \{v in V_G | delta_G(s,v) = i\}
         * Return: (R_G(s), max \{delta_G(s,v) : v in R_G(s)\}) *)
        fun BFS' (X : Set.set, F : Set.set, i : int) =
          if (Set.size F = 0) then (X, i)
          else let
            val X' = Set.union (X, F)
            val F' = Set.difference (N G F, X')
            in
            BFS'(X', F', i+1)
          end
        in
        BFS'(Set.empty, Set.singleton s, 0)
      end
  end
```

Version 1.1
Generating a BFS Tree. The following code for generating a BFS tree represents the visited set \( X \) and frontier \( F \) as a table mapping each vertex in the visited set or frontier to their parent in the BFS tree (i.e. who visited them). The function \( \text{outEdges} \) returns the out edges of \( v \) or an empty set if \( v \) is not found. The \( N_G(F) \) function now not only returns the neighbors for every vertex \( v \in F \), but also tags each neighbor with the vertex \( v \) they came from. In particular \( \text{tagNeighbors} \) tags all neighbors with \( v \), and then a \( \text{Table.reduce} \) is used to merge all the tables of tagged neighbor. The \text{merge} used in the reduce takes the first argument if there is a collision.

```ml
functor TableBFSTree(Table : TABLE) =
  struct
    structure Set = Table.Set
    type vertex = Table.key
    type graph = Set.set Table.table
    type 'a table = 'a Table.table
    type set = Set.set
    type parentsTable = vertex table
    fun merge(A,B) = Table.merge (fn (a,b) => a) (A,B)
    fun outEdges (G : graph) (v : vertex) =
      case (Table.find G v) of
        NONE => Set.empty
      | SOME(ngh) => ngh
    (* Return neighbors tagged with where they come from *)
    fun N (G : graph) (F : set) =
      let
        fun tagNeighbors v = Table.tabulate (fn _ => v) (outEdges G v)
        val ngh = Table.tabulate tagNeighbors F
      in
        Table.reduce merge (Table.empty()) ngh
      end
    fun bfsTree (G :graph) (s : vertex) =
      let
        fun BFS(X : parentsTable, F : parentsTable) =
          if (Table.size F = 0) then X
          else let
              val X' = merge(X,F)
              val Ngh = N G (Table.domain F)
              val F' = Table.erase(Ngh, Table.domain X')
            in BFS(X', F') end
        in
          BFS(Table.empty(), Table.singleton(s,s))
        end
  end
```

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