IA Algorithms

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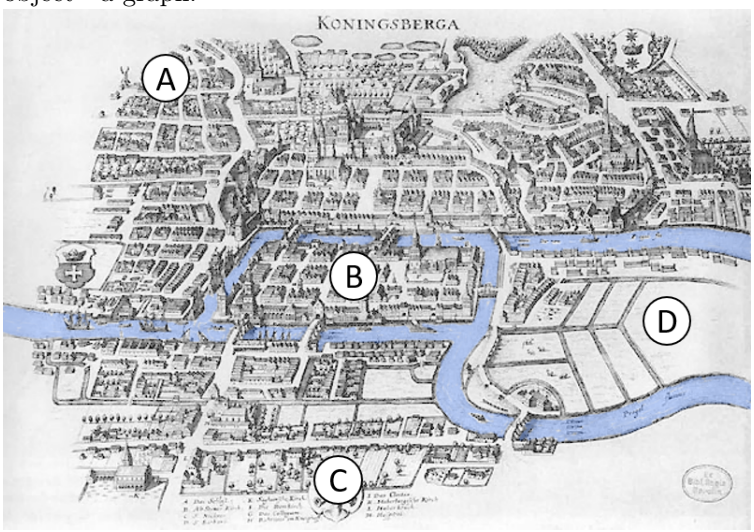
Contents

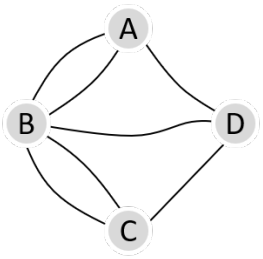
5. Graphs

5.1. Notation and representation

A great many algorithmic questions are about entities and the connections between them. Graphs are how we describe them. A graph is a set of *vertices* (or nodes, or locations) and *edges* (or connections, or links) between them.

Example. Leonard Euler in Königsberg, 1736, posed the question "Can I go for a stroll around the city on a route that crosses earch bridge exactly once?" He proved the answer was 'No'. His innovation was to turn this into a precise mathematical question about a simple discrete object—a graph.

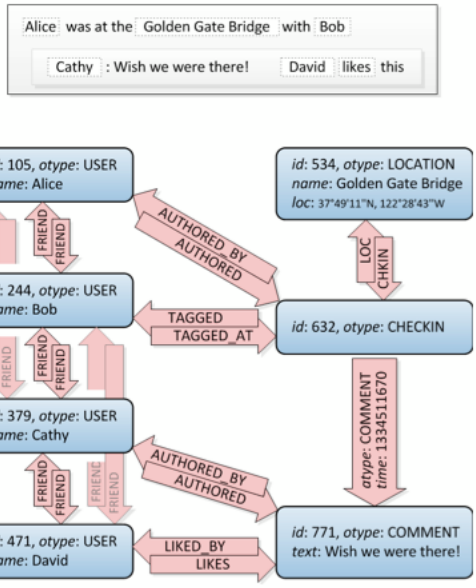





```
g = {'A': ['B', 'B', 'D'],
     'B': ['A', 'A', 'C', 'C', 'D'],
     'C': ['B', 'B', 'D'],
     'D': ['A', 'B', 'C']}
```

Example. Facebook's underlying data structure is a graph. Vertices are used to represent users, locations, comments, check-ins, etc. From the Facebook documentation,

It's up to the programmer to decide what counts as a vertex and what counts as an edge. Why do you think Facebook made CHECKIN a type of vertex, rather than an edge from a USER to a LOCATION?



Example. OpenStreetMap represents its map as XML, with nodes and ways. In some parts of the city, this data is very fine-grained. The more vertices and edges there are, the more

space it takes to store the data, and the slower the algorithms run. Later in this course we will discuss geometric algorithms which could be used to simplify the graph while keeping its basic shape.

```
<osm version="0.6" generator="Overpass API">
  <node id="687022827" user="François Guerraz"
        lat="52.2082725" lon="0.1379459" />
  <node id="687022823" user="bigalxyz123"
        lat="52.2080972" lon="0.1377715" />
  <node id="687022775" user="bigalxyz123"
        lat="52.2080032" lon="0.1376761" >
    <tag k="direction" v="clockwise"/>
    <tag k="highway" v="mini_roundabout"/>
  </node>
  <way id="3030266"  user="urViator">
    <nd ref="687022827"/>
    <nd ref="687022823"/>
    <nd ref="687022775"/>
    <tag k="cycleway" v="lane"/>
    <tag k="highway" v="primary"/>
    <tag k="name" v="East Road"/>
    <tag k="oneway" v="yes"/>
  </way>
...
</osm>
```

DEFINITIONS

Some notation for describing graphs. A *graph* is a collection of vertices, with edges between them. Write a graph as $g = (V, E)$ where V is the set of vertices and E the set of edges.

In this course we won't allow multiple edges between a pair of nodes (such as Euler used in his graph of Königsberg bridges).

- A graph may be *directed* or *undirected*;

$$\begin{aligned} &\text{in a directed graph,} && v_1 \to v_2 \quad \text{is the edge from } v_1 \text{ to } v_2 \\ &\text{in an undirected graph,} && v_1 \leftrightarrow v_2 \quad \text{is the edge between } v_1 \text{ and } v_2. \end{aligned}$$

- The *neighbours* of a vertex v are the vertices you reach by following an edge from v,

$$\begin{aligned} &\text{in a directed graph,} && \text{neighbours}(v) = \{w \in V \,:\, v \to w\} \\ &\text{in an undirected graph,} && \text{neighbours}(v) = \{w \in V \,:\, v \leftrightarrow w\}. \end{aligned}$$

Paths are allowed to visit the same vertex more than once

- A *path* is a sequence of vertices connected by edges,

$$\begin{aligned} &\text{in a directed graph,} && v_1 \to v_2 \to \cdots \to v_k \\ &\text{in an undirected graph,} && v_1 \leftrightarrow v_2 \leftrightarrow \cdots \leftrightarrow v_k. \end{aligned}$$

- A *cycle* is a path from a vertex back to itself, i.e. a path where $v_1 = v_k$.

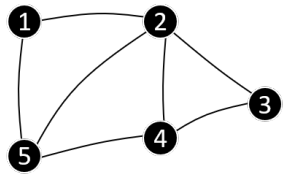
There are some special types of graph that we'll look at in more detail later.

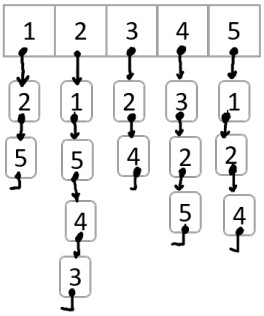
- A *directed acyclic graph* or DAG is a directed graph without any cycles. They're used all over computer science. We'll study some properties of DAGs in Section 6.6.
- An undirected graph is *connected* if for every pair of vertices there is a path between them. A *forest* is an undirected acyclic graph. A *tree* is a connected forest. We'll study algorithms for finding trees and forests in Sections 6.4–6.5.

It sounds perverse to define a tree to be a type of forest! But you need to get used to reasoning about algorithms directly from definitions, rather than from your hunches and instinct; and a deliberately perverse definition can help remind you of this.

REPRESENTATION

Here are two standard ways to store graphs in computer code: as an array of *adjacency lists*, or as an *adjacency matrix*. The former takes space $O(V + E)$ and the latter takes space $O(V^2)$, so your choice should depend on the *density* of the graph, density $= E/V^2$. (Note: V and E are sets, so we should really write $O(|V| + |E|)$ etc., but it's conventional to drop the $|\cdot|$.)





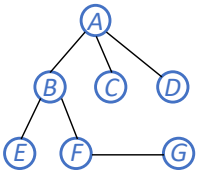
	1	**2**	**3**	**4**	**5**
1	0	1	0	0	1
2	1	0	1	1	1
3	0	1	0	1	0
4	0	1	1	0	1
5	1	1	0	1	0

5.2. Depth-first search

A common task is traversing a graph and doing some work at each vertex. For example, a web crawler for a search engine visits every page it can find, and at each page the work is to process the text to add to its search index, then extract all the links in order to find new pages.

GENERAL IDEA: LIKE TRAVERSING A TREE

It's easy to explore a tree, using recursion. If we call visit_tree(B, None) on the tree shown here then we'll see it visit B, E, F, A, C, D, G (or perhaps some other order depending on the order of each vertex's neighbours).



We defined *tree* to mean 'undirected connected acyclic graph'. This tree is drawn as if to suggest that A is the root, but because we defined it to be undirected there is actually no root.

```
# Visit all vertices in the subtree rooted at v
def visit_tree(v, v_parent):
    print "visiting", v
    for w in v.neighbours:
        # Only visit v's children, not its parent
        if w != v_parent:
            visit_tree(w, v)
```

DFS IMPLEMENTATION 1: USING RECURSION

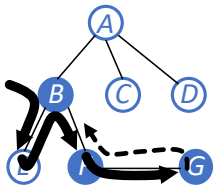
Depth-first search uses the same idea as traversing a tree. But for an arbitrary graph there might be edges that lead from a node back to parts of the graph that we've already visited, so we need to explicitly mark which vertices have already been visited, so that we don't get stuck in an infinite loop.

```
# Visit all vertices reachable from s
def dfs_recurse(g, s):
    for v in g.vertices:
        v.visited = False
    visit(s)

def visit(v):
    v.visited = True
    for w in v.neighbours:
        if not w.visited:
            visit(w)
```

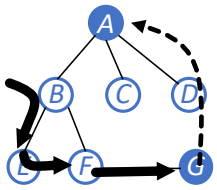
DFS IMPLEMENTATION 2: WITH A STACK

Now a second implementation. The recursive implementation backtracks along vertices it has already visited, to find the next unvisited neighbour. Instead of backtracking, we can just keep a record of which vertices are waiting to be explored, and jump straight to the next one in the list. We'll use a Stack, a Last-In-First-Out data structure, to store this list: this way we'll visit children before returning to distant cousins.

There is a subtle difference between dfs and dfs_recurse — they don't visit vertices in the same order as each other. Example Sheet 5 asks you to consider this further.



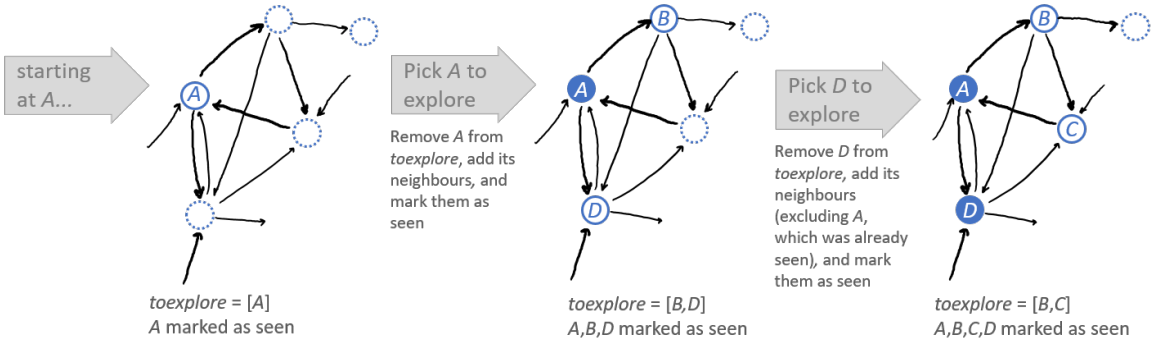
dfs_recurse



dfs using a Stack

```
# Visit all vertices reachable from s
def dfs(g, s):
```

```
3       for v in g.vertices:
4           v.seen = False
5       toexplore = Stack([s])    # a Stack initially containing a single element
6       s.seen = True
7
8       while not toexplore.is_empty():
9           v = toexplore.popright()    # Now visiting vertex v
10          for w in v.neighbours:
11              if not w.seen:
12                  toexplore.pushright(w)
13                  w.seen = True
```



ANALYSIS

In dfs, (a) line 4 is run for every vertex which takes $O(V)$; (b) lines 8–9 are run at most once per vertex, since the seen flag ensures that each vertex enters toexplore at most once, so the running time is $O(V)$; (c) lines 10 and below are run for every edge out of every vertex that is visited, which takes $O(E)$. Thus the total running time is $O(V + E)$.

The dfs_recurse algorithm also has running time $O(V + E)$. To see this, (a) line 4 is run once per vertex, (b) line 8 is run at most once per vertex, since the visited flag ensures that visit(v) is run at most once per vertex; (c) lines 9 and below are run for every edge out of every vertex visited.

* * *

Pay close attention to the clever trick in analysing the running time. We didn't try to build up some complicated recursive formula about the running time of each call to visit, or to reason about when which part of the graph was put on the stack. Instead we used mathematical reasoning to bound the total number of times that a vertex could possibly be processed during the entire execution. This is called *aggregate analysis*, and we'll see many more examples throughout the course.

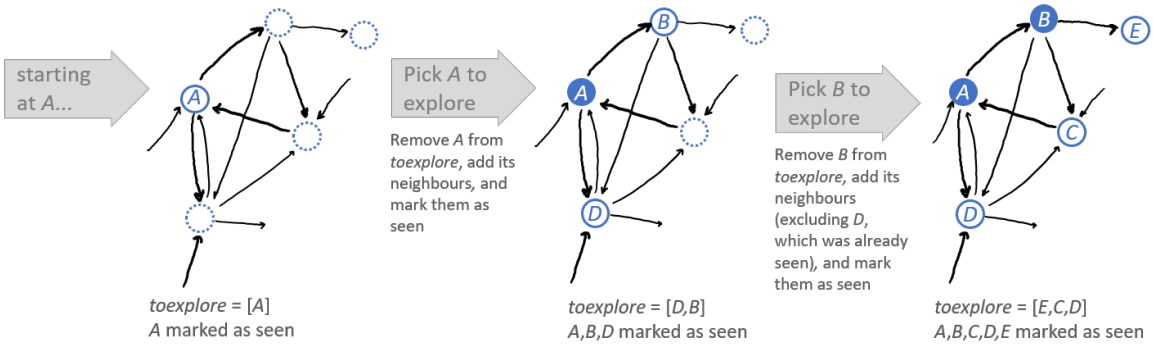
The recursive implementation uses the language's call stack, rather than our own data structure. Recursive algorithms are sometimes easier to reason about, and we'll use the recursive implementation as part of a proof in Section 6.6.

5.3. Breadth-first search

A common task is finding paths in a graph. With a tiny tweak to the depth-first search algorithm, we can find shortest paths.

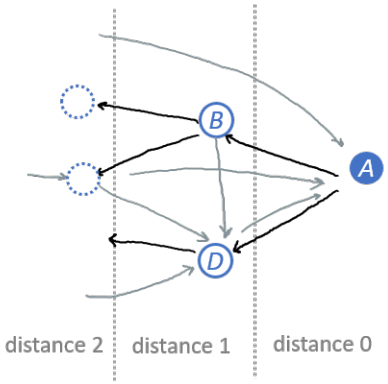
GENERAL IDEA

Suppose we proceed as for dfs on page 4, but use a Queue (pushing new vertices on the left, popping them from the right) instead of a Stack to store the list of vertices waiting to be explored.



To understand what's special about the Queue, here's the same graph but redrawn so that vertex A is on the right, and the other vertices are arranged by their distance from A. (The *distance* from one vertex v to another vertex w is the length of the shortest path from v to w.) By using a Queue for toexplore, we visit every node at distance d before visiting anything at distance $d+1$, i.e. we explore the graph in order of distance from the start vertex.

If you rotate this diagram 90°anticlockwise, you can see why the algorithm is called 'breadth-first search'.

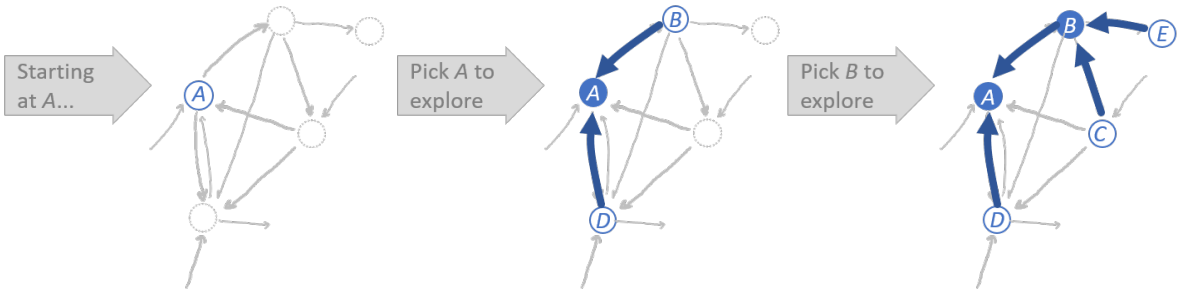


IMPLEMENTATION

The following code is almost identical to dfs. The only difference is that it uses a Queue instead of a Stack.

```
# Visit all the vertices in g reachable from start vertex s
def bfs(g, s):
    for v in g.vertices:
        v.seen = False
    toexplore = Queue([s])  # a Queue initially containing a single element
    s.seen = True

    while not toexplore.is_empty():
        v = toexplore.popright()   # Now visiting vertex v
        for w in v.neighbours:
            if not w.seen:
                toexplore.pushleft(w)
                w.seen = True
```

We can adapt this code to find a path between a pair of nodes: we just need to keep track of how we discovered each vertex. At every vertex we'll store a come_from arrow, pointing to a vertex one hop closer to the start vertex. Here's a picture, then the code.



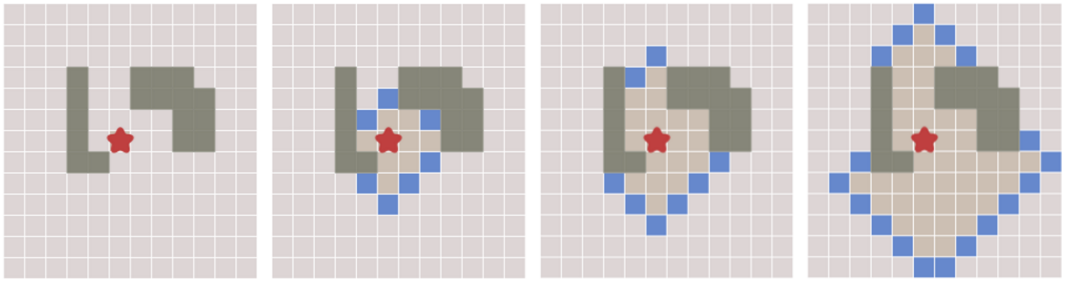

```
# Find a path from s to t, if one exists
def bfs_path(g, s, t):
    for v in g.vertices:
        v.seen = False
        v.come_from = None
    s.seen = True
    toexplore = Queue([s])

    # Traverse the graph, visiting everything reachable from s
    while not toexplore.is_empty():
        v = toexplore.popright()
        for w in v.neighbours:
            if not w.seen:
                toexplore.pushleft(w)
                w.seen = True
                w.come_from = v

    # Reconstruct the full path from s to t, working backwards
    if t.come_from is None:
        return None  # there is no path from s to t
    else:
        path = [t]
        while path[0].come_from != s:
            path.prepend(path[0].come_from)
        path.prepend(s)
        return path
```

ANALYSIS

The bfs algorithm has running time $O(V+E)$, based on exactly the same analysis as for dfs in section 5.2.

* * *

Here is another way to think of the bfs algorithm: keep track of the 'disc' of vertices that are distance $\leq d$ from the start, then grow the disc by adding the 'frontier' of vertices at distance $d+1$, and so on. What's magic is that the bfs algorithm does this implicitly, via the Queue, without needing an explicit variable to store d.



In this illustration[1], we're running bfs starting from the blob in the middle. The graph has one vertex for each light grey grid cell, and edges between adjacent cells, and the black cells in the left hand panel are impassable. The next three panels show some stages in the expanding frontier.

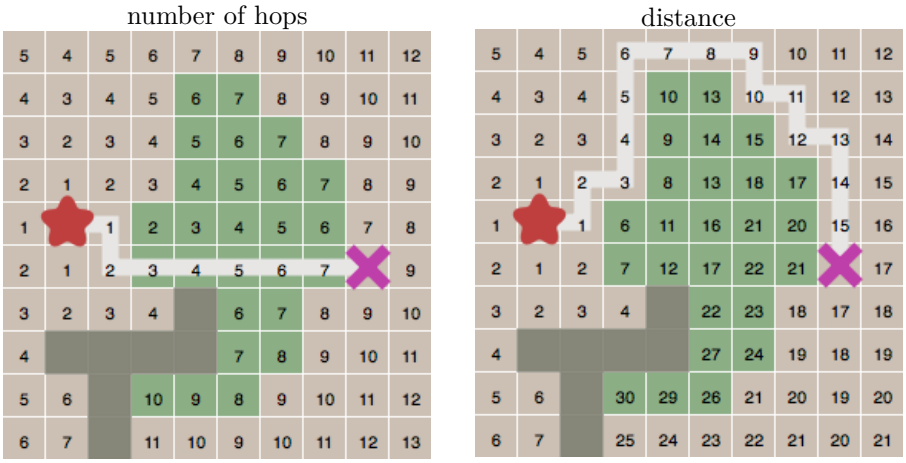
[1]These pictures are taken from the excellent Red Blob Games blog, `http://www.redblobgames.com/pathfinding/a-star/introduction.html`

5.4. Dijkstra's algorithm

In many applications it's natural to use graphs where each edge is labelled with a cost, and to look for paths with minimum cost. For example, suppose the graph's edges represent road segments, and each edge is labelled its travel time: how do we find the quickest route between two locations?

This is called the *shortest path problem*. We'll use the terms *cost* and *distance* interchangeably, and write 'distance from v_1 to v_2' to mean 'the cost of a minimum-cost path from v_1 to v_2'.

Here's an illustration[2]. These pictures show two possible paths between the blob and the cross. The left hand picture shows the number of hops from the blob; the right picture shows the distance from the blob. Here, the darkest cells can't be crossed, light cells cost 1 to cross, and darker cells cost 5.

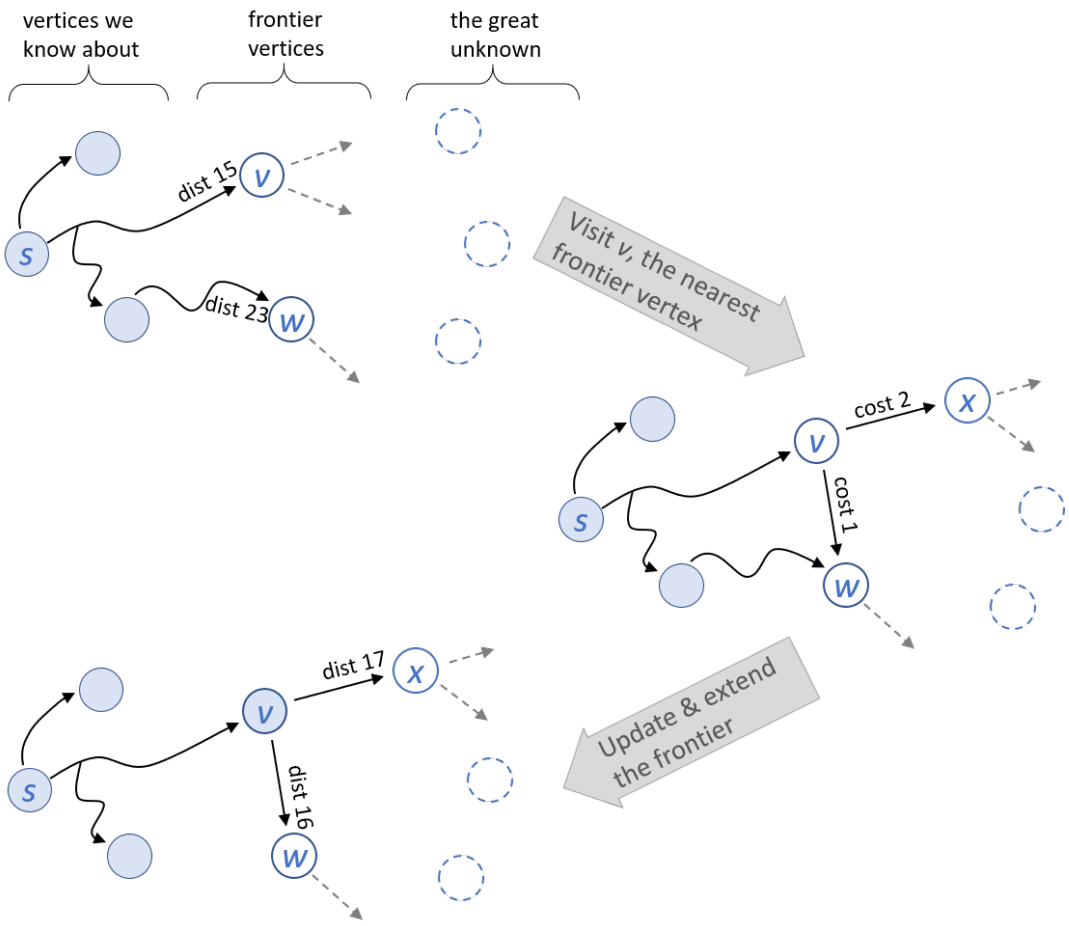


GENERAL IDEA

In breadth-first search, we visited vertices in order of how many hops they are from the start vertex. Now, let's visit vertices in order of distance from the start vertex. We'll keep track of a frontier of vertices that we're waiting to explore (i.e. the vertices whose neighbours we haven't yet examined). We'll keep the frontier vertices ordered by distance, and at each iteration we'll pick the next closest.

We might end up coming across a vertex multiple times, with different costs. If we've never come across it, just add it to the frontier. If we've come across it previously and our new path is shorter than the old path, then update its distance.

[2]Pictures taken from the Red Blob Games blog, `http://www.redblobgames.com/pathfinding/a-star/introduction.html`



PROBLEM STATEMENT

What goes wrong in the algorithm below, and in the proof, if there are negative costs? Try to work it out yourself, before reading the answer in Section 5.6.

Given a directed graph where each edge is labelled with a cost ≥ 0, and a start vertex s, compute the distance from s to every other vertex.

IMPLEMENTATION

This algorithm was invented in 1959 and is due to Dijkstra[3] (1930–2002), a pioneer of computer science.

See Section 4.8 for a definition of PriorityQueue. It supports inserting items, decreasing the key of an item, and extracting the item with smallest key.

Line 5 declares that toexplore is a PriorityQueue in which the key of an item v is v.distance. Line 11 iterates through all the vertices w that are neighbours of v, and retrieves the cost of the edge $v \to w$ at the same time.

```
1  def dijkstra(g, s):
2      for v in g.vertices:
3          v.distance = ∞
4      s.distance = 0
5      toexplore = PriorityQueue([s], sortkey = lambda v: v.distance)
6
7      while not toexplore.isempty():
8          v = toexplore.popmin()
9          # Assert: v.distance is the true shortest distance from s to v
10         # Assert: v is never put back into toexplore
11         for (w, edgecost) in v.neighbours:
12             dist_w = v.distance + edgecost
```

[3]Dijkstra was an idiosyncratic character famous for his way with words. Some of his sayings: "The question of whether Machines Can Think [...] is about as relevant as the question of whether Submarines Can Swim." And "If you want more effective programmers, you will discover that they should not waste their time debugging, they should not introduce the bugs to start with."

```
13              if dist_w < w.distance:
14                  w.distance = dist_w
15                  if w in toexplore:
16                      toexplore.decreasekey(w)
17                  else:
18                      toexplore.push(w)
```

Although we've called the variable v.distance, we really mean "shortest distance from s to v that we've found so far". It starts at ∞ and it decreases as we find new and shorter paths to v. Given the assertion on line 10, we could have coded this algorithm slightly differently: we could put all nodes into the priority queue in line 5, and delete lines 15, 17, and 18. It takes some work to prove the assertion...

ANALYSIS

Running time. The running time depends on how the PriorityQueue is implemented. Later in the course, we'll describe an implementation called the Fibonacci heap which for n items has $O(1)$ running time for both push() and decreasekey() and $O(\log n)$ running time for popmin(). Line 8 is run at most once per vertex (by the assertion on line 10), and lines 12–18 are run at most once per edge. So Dijkstra has running time $O(E + V \log V)$, when implemented using a Fibonacci heap.

Theorem (Correctness). *The dijkstra algorithm terminates. When it does, for every vertex v, the value v.distance it has computed is equal to the true distance from s to v. Furthermore, the two assertions are true.*

Proof (of Assertion 9). Suppose this assertion fails at some point in execution, and let v be the vertex for which it first fails. Consider a shortest path from s to v. (This means the Platonic mathematical object, *not* a computed variable.) Write this path as

$$s = u_1 \to \cdots \to u_k = v$$

Pay close attention to whether you're dealing with abstract mathematical statements (which can be stated and proved even without an algorithm), or if you're reasoning about program execution.

Let u_i be the first vertex in this sequence which has not been popped from toexplore so far at this point in execution (or, if they have all been popped, let $u_i = v$). Then,

$$\begin{aligned}
&\text{distance}(s \text{ to } v) \\
&\quad < v.\text{distance} && \text{since the assertion failed} \\
&\quad \le u_i.\text{distance} && \text{since toexplore is a PriorityQueue which had both } u_i \text{ and } v \\
&\quad \le u_{i-1}.\text{distance} + \text{cost}(u_{i-1} \to u_i) && \text{by lines 13–18 when } u_{i-1} \text{ was popped} \\
&\quad = \text{distance}(s \text{ to } u_{i-1}) + \text{cost}(u_{i-1} \to u_i) && \text{assertion didn't fail at } u_{i-1} \\
&\quad \le \text{distance}(s \text{ to } v) && \text{since } s \to \cdots u_{i-1} \to u_i \text{ is on a shortest path } s \text{ to } v.
\end{aligned}$$

This is a contradiction, therefore the premise (that Assertion 9 failed at some point in execution) is false.

Proof (of Assertion 10). Once a vertex v has been popped, Assertion 9 guarantees that v.distance = distance(s to v). The only way that v could be pushed back into toexplore is if we found a shorter path to v (on line 13) which is impossible.

Rest of proof. Since vertices can never be re-pushed into toexplore, the algorithm must terminate. At termination, all the vertices that are reachable from s must have been visited, and popped, and when they were popped they passed Assertion 9. They can't have had v.distance changed subsequently (since it can only ever decrease, and it's impossible for it to be *less* than the true minimum distance, since the algorithm only ever looks at legitimate paths from s.) □

* * *

The proof technique was *proof by induction*. We start with an ordering (the order in which vertices were popped during execution), we assume the result is true for all earlier vertices,

and we prove it true for the next. For some graph algorithms it's helpful to order differently, e.g. by distance rather than time. Whenever you use this proof style, make sure you say explicitly what your ordering is.

5.5. Algorithms and proofs

According to Dijkstra, "Programming is one of the most difficult branches of applied mathematics; the poorer mathematicians had better remain pure mathematicians."[4] Here is an exam question about Dijsktra's algorithm, and a selection of mangled proofs.

> Let dijkstra_path(g, s, t) be an implementation of Dijkstra's shortest path algorithm that returns the shortest path from vertex s to vertex t in a graph g. Prove that the implementation can safely terminate when it first encounters vertex t.

Bad answer 1. Dijkstra's algorithm performs a depth-first search on the graph, storing a frontier of all unexplored vertices that are neighbours to explored vertices.

Each time it chooses a new vertex v to explore, from the frontier of unexplored vertices, it chooses the one that will have the shortest distance from the start s, based on the edge weight plus the distance from its already explored neighbour.

Given that no other vertex in the frontier is closer to s, and that this new vertex v has yet to be explored, when v is explored it must have been via the shortest path from s to v.

Hence, when t is first encountered, it must have been found via its shortest path and the program can safely terminate.

The claim here is "it chooses the one that will have the shortest distance". There are two distances here: (a) v.distance, the quantity computed and updated in the course of the algorithm, and (b) distance(*s to v*)*, the true mathematical distance. The whole point of proof of Dijkstra's algorithm is to establish that these two distances agree, at the instant a vertex is popped.*

This Bad Answer muddles the two distances. It assumes that the computed distance, which governs popping order, is equal to mathematical distance.

Finally, it is bad sign to claim that Dijkstra's algorithm performs depth-first search. It does nothing of the sort!

Bad answer 2. At the moment when the vertex t is popped from the priority queue, it has to be the vertex in the priority queue with the least distance from s. This means that any other vertex in the priority queue has distance $\geq$ that for t. Since all edge weights in the graph are ≥ 0, any path from s to t via anything still in the priority queue will have distance $\geq$ that of the distance from s to t when t is popped, thus the distance to t is correct when t is popped.

This is another example of wishful thinking, like the previous answer. The first sentence only makes sense if it is referring to distances as computed by the algorithm. The "any path" sentence needs to argue about "the true distance of any path from s to t", but it only argues about the distances as computed; this proof hasn't established whether those computed distances are correct.

Bad answer 3. In Dijkstra's algorithm we add vertices to a min priority queue sorted by the shortest distance to them from the start vertex s. We then repeatedly pop the minimum element in the priority queue.

Assume that at the time we pop t, there is a shorter path to it than the one we just found. If that is the case, then there is some vertex x that immediately precedes t in the shorter path.

However, this x cannot exist, as if it did it would have been popped from the frontier before t (path $s \rightsquigarrow x$ must be shorter than the path $s \rightsquigarrow t$) and is already part of the path being considered. We reach a contradiction, so the assumption that there is a shorter path than the one found must be false.

[4] EWD 498: How do we tell truths that might hurt? `https://www.cs.utexas.edu/users/EWD/ewd04xx/EWD498.PDF`

This is another example of wishful thinking, assuming that computed distances are equal to true distances. The vertex x is chosen by considering a true (mathematical) shorter path to t. What if, at the time we pop t, the computed distance to x is incorrect? Then the argument about "would have been popped before" wouldn't hold.

Bad answer 4. Assume that upon termination the path to t is suboptimal. Let v be the vertex which is first in the computed path that is not on the shortest path. Let u_i be the node on the shortest path that should have been chosen instead of v.

$$s = u_1 \to u_2 \to \cdots \to u_{i-1} \to v \to \cdots \to t \quad \text{(computed path)}$$
$$s = u_1 \to u_2 \to \cdots \to u_{i-1} \to u_i \to \cdots \to t \quad \text{(true shortest path)}$$

Since v is not optimal,

$$\begin{aligned}
&\text{distance}(s \text{ to } v) < v.\mathsf{distance} \quad \text{since } v \text{ is not optimal} \\
&\quad \leq \text{distance}(s \text{ to } u_{i-1}) + \text{cost}(u_{i-1} \to v) \quad \text{as it didn't fail at } u_{i-1} \\
&\quad \leq \text{distance}(s \text{ to } u_{i-1}) + \text{cost}(u_{i-1} \to u_i) \quad \text{as } v \text{ was chosen over } u_i \text{ in priority queue} \\
&\quad \leq \text{distance}(s \text{ to } v) \quad \text{as } u_i \text{ is on the shortest path to } v.
\end{aligned}$$

We have proved that distance(s to v) $<$ distance(s to v), a contradiction, hence the path must be the shortest.

This Bad Answer makes the same error of wishful thinking as the others, but it is wrapped up in fancier notation. It jumps from "v should not have been chosen" to "v is not optimal" to "v.distance is larger than the true distance", without explaining the link between these three concepts.

* * *

The (correct) proof of Dijkstra's algorithm has two key ingredients:

- It needs to establish that when a vertex is popped, its computed distance is equal to the true (mathematical) distance. To do this, it considers the *first* instant during execution at which this fails — this means we can assume that all previously popped vertices are correct. (Formally, the proof is an induction on vertices ordered by when they are popped.) Any proof should carefully distinguish "program state at a particular instant during execution" from "mathematical facts which are always true".
- Dijkstra's algorithm only works if all costs are ≥ 0, as we'll see in the next section. Any proof which doesn't reference this must be incorrect.

5.6. Bellman-Ford

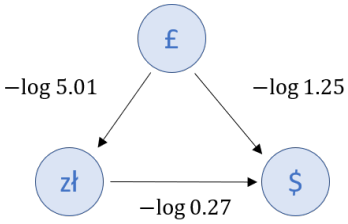
Now for a new wrinkle: we'll allow edges to have negative costs.

We'll use the term *weight* rather than cost of an edge, and *minweight* rather than distance between two vertices, and *minimal weight path* rather than shortest path. (The words 'cost' and 'distance' suggests positive numbers, and so they give us bad intuition for graphs with negative costs.) Our goal is as before to find minimal weight paths from some start vertex.

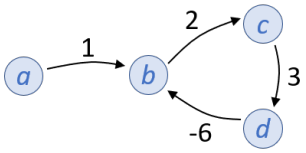
Example (Planning problems). Consider a graph in which vertices represent the states that an agent can be in, and edges represent actions that take it from one state to another. Actions can have costs or rewards. The agent's goal is to find the best sequence of actions to achieve some end state.

Here's an application: currency exchange. Suppose I start with £1 and I want to convert it to \$, perhaps via some intermediate currencies. Let there be a vertex for each currency — vertex v represents the state "my money is held in currency v". Let edges represent exchanges we can perform: if 1 unit of v_1 can be exchanged for x units of v_2, we'll put an edge from v_1 to v_2 with weight $-\log x$. The graph below depicts possible exchanges £1 for \$1.25, £1 for 5.01 zł, and 1 zł for \$0.27.

The weight of the £→zł→\$ path is $-\log 5.01 - \log 0.27 = -\log(5.01 * 0.27) = -\log 1.35$, and the weight of the direct £→\$ edge is $-\log 1.25$. Because of the log, the path weight corresponds to the net exchange rate, and because of the minus sign the minimal weight path corresponds to the most favourable sequence of exchanges.



Example (Negative cycles). What's the minimum weight from a to b in the graph below? By going around $b \to c \to d \to b$ again and again, the weight of the path goes down and down. This is referred to as a *negative weight cycle*, and we'd say that the minimum weight from a to b is $-\infty$.



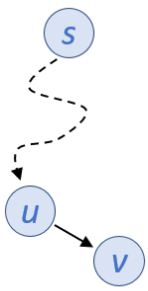
$a \to b$: weight 1
$a \to b \to c \to d \to b$: weight 0
$a \to b \to c \to d \to b \to c \to d \to b$: weight -1

GENERAL IDEA

Dijsktra's algorithm can fail on graphs with negative edge weights. *Before continuing, you should (1) work out what Dijkstra's algorithm would actually do, when run on the above graph with a negative weight cycle, (2) identify how the proof of Disjkstra's algorithm fails.*

But the update step at the heart of Dijkstra's algorithm, lines 13–14, it still sound. Let's restate it. If we've found a path from s to u, call it $s \rightsquigarrow u$, and if there is an edge $u \to v$, then $s \rightsquigarrow u \to v$ is a path from s to v. If we store the minimum weight path we've found so far in the variable minweight, then the obvious update is

$$\begin{aligned} &\text{if } v.\text{minweight} > u.\text{minweight} + \text{weight}(u \to v) : \\ &\quad \text{let } v.\text{minweight} = u.\text{minweight} + \text{weight}(u \to v) \end{aligned}$$



This update rule is known as *relaxing the edge* $u \to v$.

Dijkstra's algorithm visits vertices in order of their distance from a given start vertex, and at every vertex v it visits it relaxes all of v's outgoing edges. The idea of the Bellman-Ford algorithm is to forget about ordering, and simply to keep applying relaxation to all

edges in the graph, over and over again, updating "best weight from s to v found so far" if a path via u gives a lower weight. The magic is that we only need to apply it a fixed number of times.

PROBLEM STATEMENT

Given a directed graph where each edge is labelled with a weight, and a start vertex s, (i) if the graph contains no negative-weight cycles reachable from s then for every vertex v compute the minimum weight from s to v; (ii) otherwise report that there is a negative weight cycle reachable from s.

IMPLEMENTATION

In this code, lines 8 and 12 iterate over all edges in the graph, and c is the weight of the edge $u \to v$. The assertion in line 10 refers to the true minimum weight among all paths from s to v, which the algorithm doesn't know yet; the assertion is just there to help us reason about how the algorithm works, not something we can actually test during execution.

```
1  def bf(g, s):
2      for v in g.vertices:
3          v.minweight = ∞ # best estimate so far of minweight from s to v
4      s.minweight = 0
5
6      repeat len(g.vertices)−1 times:
7          # relax all the edges
8          for (u,v,c) in g.edges:
9              v.minweight = min(u.minweight + c, v.minweight)
10             # Assert v.minweight >= true minimum weight from s to v
11
12     for (u,v,c) in g.edges:
13         if u.minweight + c < v.minweight:
14             throw "Negative−weight cycle detected"
```

Lines 12–14 say, in effect, "If the answer we get after $V-1$ rounds of relaxation is different to the answer after V rounds, then there is a negative-weight cycle; and vice versa."

ANALYSIS

The algorithm iterates over all the edges, and it repeats this V times, so the overall running time is $O(VE)$.

Theorem. *The algorithm correctly solves the problem statement. In case (i) it terminates successfully, and in case (ii) it throws an exception in line 14. Furthermore the assertion on line 10 is true.*

Proof (of assertion on line 10). Write $w(v)$ for the true minimum weight among all paths from s to v, with the convention that $w(v) = -\infty$ if there is a path that includes a negative-weight cycle. The algorithm only ever updates v.minweight when it has a valid path to v, therefore the assertion is true.

Proof for case (i). Pick any vertex v, and consider a minimal-weight path from s to v. Let the path be

$$s = u_0 \to u_1 \to \cdots \to u_k = v.$$

Consider what happens in successive iterations of the main loop, lines 8–10.

- Initially, u_0.minweight is correct, i.e. equal to $w(s)$ which is 0.
- After one iteration, u_1.minweight is correct. Why? If there were a lower-weight path to u_1, then the path we've got here couldn't be a minimal-weight path to v.

- After two iterations, $u_2.\mathsf{minweight}$ is correct.
- and so on...

We can assume (without loss of generality) that this path has no cycles—if it did, the cycle would have weight ≥ 0 by assumption, so we could cut it out. So it has at most $|V|-1$ edges, so after $|V|-1$ iterations $v.\mathsf{minweight}$ is correct.

Thus, by the time we reach line 12, all vertices have the correct $\mathsf{minweight}$, hence the test on line 13 never goes on to line 14, i.e. the algorithm terminates without an exception.

Proof of (ii). Suppose there is a negative-weight cycle reachable from s,

$$s \to \cdots \to v_0 \to v_1 \to \cdots \to v_k \to v_0$$

where

$$\text{weight}(v_0 \to v_1) + \cdots + \text{weight}(v_k \to v_0) < 0.$$

If the algorithm terminates without throwing an exception, then all these edges pass the test in line 13, i.e.

$$\begin{aligned} v_0.\mathsf{minweight} + \text{weight}(v_0 \to v_1) &\geq v_1.\mathsf{minweight} \\ v_1.\mathsf{minweight} + \text{weight}(v_1 \to v_2) &\geq v_2.\mathsf{minweight} \\ &\vdots \\ v_k.\mathsf{minweight} + \text{weight}(v_k \to v_0) &\geq v_0.\mathsf{minweight} \end{aligned}$$

Putting all these equations together,

$$v_0.\mathsf{minweight} + \text{weight}(v_0 \to v_1) + \cdots + \text{weight}(v_k \to v_0) \geq v_0.\mathsf{minweight}$$

hence the cycle has weight ≥ 0. This contradicts the premise—so at least one of the edges must fail the test in line 13, and so the exception will be thrown. □

5.7. Dynamic programming

Dynamic programming means figuring out how to express a problem in terms of easier subproblems. Richard Bellman (1920–1984) invented dynamic programming in order to solve planning problems, which, as we saw in section 5.6, can be thought of as finding minimal weight paths on a graph.

We'll start with Bellman's formulation of dynamic programming for solving planning problems, and then we'll see how to turn it into an algorithm.

GENERAL IDEA

Consider a graph in which vertices represent the states that an agent can be in, and edges represent actions that take it from one state to another. Actions have weights which can be either positive (costs) or negative (rewards). The goal is to find a minimal weight sequence of actions to achieve some end state, within a specified time horizon. The time horizon is crucial: we'll break the problem into easier subproblems based on how much time the agent has left.

Define the *value function* $F_T(v,t)$ to be the minimal weight for achieving a target end-state at timestep T, starting from state v at timestep t. The terminal condition is

$$F_T(v,T) = \begin{cases} 0 & \text{if } v \text{ is the target end-state} \\ \infty & \text{otherwise.} \end{cases}$$

the minimum over an empty set is taken to be ∞

The dynamic programming equation (called the Bellman equation) is

$$F_T(v,t) = \min_{w:v\to w} \Big\{ \text{weight}(v \to w) + F_T(w, t+1) \Big\}.$$

We can simply iterate backwards from $t = T-1$ to $t = 0$ to find the action to take at timestep 0.

To turn the Bellman equation into an algorithm for finding minimal weight paths, there are two tricks. The first is some clever analysis to show that $T = |V| - 1$ is sufficient to find a minimal weight path between any pair of vertices, the same analysis we used when proving Bellman–Ford case (i) correct in section 5.6. The second trick is some nifty notation that lets us do the dynamic programming iteration using matrix maths.

PROBLEM STATEMENT

Given a directed graph where each edge is labelled with a weight, and assuming it contains no negative-weight cycles, then for every pair of vertices compute the weight of the minimal-weight path between those vertices.

IMPLEMENTATION

The mathematics comes out neater if we tweak the planning problem slightly, to allow the agent a zero-weight action "stay where you are" from every state. The minimum weight of going from i to j in $\le \ell$ steps in the original problem, is thus equal to the minimum weight of going from i to j in exactly ℓ steps in the tweaked problem. To turn the tweaked problem into matrix equations, let $n = |V|$ be the number of vertices, and define a $n \times n$ matrix W: let W_{ij} be the weight of the action "go from state i to state j",

$$W_{ij} = \begin{cases} 0 & \text{if } i = j \\ \text{weight}(i \to j) & \text{if there is an edge } i \to j \\ \infty & \text{otherwise.} \end{cases}$$

The notation $x \wedge y$ means $\min(x, y)$.

Also, let $M_{ij}^{(\ell)}$ be minimum weight of going from i to j in exactly ℓ steps,

$$M_{ij}^{(1)} = W_{ij}$$
$$M_{ij}^{(\ell)} = \min_k \Big\{ W_{ik} + M_{kj}^{(\ell-1)} \Big\}.$$

This is nothing other than matrix notation for the Bellman equation. In words, to go from i to j in ℓ steps, the agent's first step is to some next state k, and then it has to get from k to j in $\ell - 1$ steps, and it should choose its first step to minimize the total weight. We set $W_{ik} = \infty$ if there is no edge $i \to k$, to ensure that the agent does not choose an illegal first step in the graph.

Unpacking this equation from planning back to graph terminology, it says "the minimum weight path from i to j with $\leq \ell$ edges is either a path with $\leq \ell - 1$ edges, or it is the edge from i to some other vertex k followed by a path from k to j with $\leq \ell - 1$ edges."

The matrix-Bellman equation can be rewritten as

$$M_{ij}^{(\ell)} = \big(W_{i1} + M_{1j}^{(\ell-1)}\big) \wedge \big(W_{i2} + M_{2j}^{(\ell-1)}\big) \wedge \cdots \wedge \big(W_{in} + M_{nj}^{(\ell-1)}\big).$$

This is just like regular matrix multiplication

$$[A\,B]_{ij} = A_{i1}B_{1j} + A_{i2}B_{2j} + \cdots + A_{in}B_{nj}$$

except it uses $+$ instead of multiplication and $\wedge$ instead of addition. Let's write it $M^{(\ell)} = W \otimes M^{(\ell-1)}$. This nifty notation lets us write out the algorithm very concisely:

```
Let M^(1) = W
Compute M^(n-1), using M^(ℓ) = W ⊗ M^(ℓ-1)
Return M^(n-1)
```

ANALYSIS

Correctness. We constructed $M_{ij}^{(\ell)}$ to be the minimum weight from i to j among all paths with $\leq \ell$ edges. The only thing left to prove is that $\ell = n-1$ is big enough to find all minimal weight paths. Suppose there is a path from i to j with n or more edges. Since the graph has only n vertices, this path must have a cycle. By assumption this cycle has weight ≥ 0, so the path's weight will remain the same or decrease if we cut out the cycle. Therefore, for every i and j, there is a minimum weight path between them of $\leq n - 1$ edges.

Running time. As with regular matrix multiplication, it takes V^3 operations to compute $\otimes$, so the total running time is $O(V^4)$. There is a cunning trick to reduce the running time. Let's illustrate with $V = 10$. Rather than applying $\otimes$ 8 times to compute $M^{(9)}$, we can repeatedly square:

$$\begin{aligned}
M^{(1)} &= W \\
M^{(2)} &= M^{(1)} \otimes M^{(1)} \\
M^{(4)} &= M^{(2)} \otimes M^{(2)} \\
M^{(8)} &= M^{(4)} \otimes M^{(4)} \\
M^{(16)} &= M^{(8)} \otimes M^{(8)} \\
&= M^{(9)} \quad \text{as there are no negative-weight cycles.}
\end{aligned}$$

This trick gives overall running time $O(V^3 \log V)$.

* * *

There is a multitude of ways that a given planning problem can be expressed as dynamic programming. In this case, for example, we could just as well have written a backwards version,

$$M_{ij}^{(\ell)} = \min_k \Big\{ M_{ik}^{(\ell-1)} + W_{kj} \Big\}$$

i.e. to go from i to j in ℓ steps, the agent has to get to some penultimate state k in $\ell - 1$ steps, and then take the edge from k to j.

It is usually impractical to solve the Bellman equation exactly, because the number of states in a typical planning problem is combinatorially huge. Reinforcement learning[5], as used by DeepMind's AlphaGo, is an way to compute approximate solutions.

[5] See `https://blog.evjang.com/2018/08/dijkstras.html` for an excellent blog post by Eric Jang, that discusses the link between reinforcement learning and shortest paths.

5.8. Johnson's algorithm

What if we want to compute shortest paths between *all* pairs of vertices?

- Each router in the internet has to know, for every packet it might receive, where that packet should be forwarded to. Path preferences in the Internet are based on link costs set by internet service providers. Routers send messages to each other advertising which destinations they can reach and at what cost. The Border Gateway Protocol (BGP) specifies how they do this. It is a distributed path-finding algorithm, and it is a much bigger challenge than computing paths on a single machine.
- The *betweenness centrality* of an edge is defined to be the number of shortest paths that use that edge, over all the shortest paths between all pairs of vertices in a graph. (If there are n shortest paths between a pair of vertices, count each of them as contributing $1/n$.) The betweenness centrality is a measure of how important that edge is, and it's used for summarizing the shape of e.g. a social network. To compute it, we need shortest paths between all pairs of vertices.

GENERAL IDEA

If all edge weights are ≥ 0, we can just run Dijkstra's algorithm V times, once from each vertex. This has running time

$$V \cdot O(E + V \log V) = O(VE + V^2 \log V).$$

If some edge weights are < 0, we could run the dynamic programming algorithm based on Bellman's equation, which has running time

$$O(V^3 \log V).$$

Or we could run Bellman-Ford from each vertex, which would have running time

$$V \cdot O(VE) = O(V^2 E).$$

Depending on the number of edges, these may be more or less appealing. Here's a summary for two cases, $E = V - 1$ (a tree, the smallest connected graph on V vertices), and $E = V(V-1)$ (a fully connected directed graph):

	Dijkstra	dynamic prog.	Bellman-Ford
$E = V - 1$	$O(V^2 \log V)$	$O(V^3 \log V)$	$O(V^3)$
$E = V(V-1)$	$O(V^3)$	$O(V^3 \log V)$	$O(V^4)$

The Dijkstra column is best, but Dijkstra's algorithm only works if all edge weights are ≥ 0. Happily there is a clever trick, discovered by Donald Johnson in 1977, whereby we can run Bellman-Ford once, then run Dijkstra once from each vertex, then run some cleanup for every pair of vertices. The running time is therefore

$$O(VE) + O(VE + V^2 \log V) + O(V^2) = O(VE + V^2 \log V).$$

It's as if we cope with negative edge weights for free!

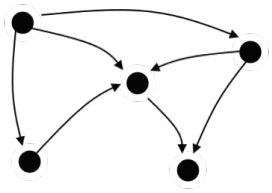
The algorithm works by constructing an extra 'helper' graph, running a computation in it, and applying the results of the computation to the original problem. This is a common pattern, and we'll see it again in Section 6.3.

PROBLEM STATEMENT

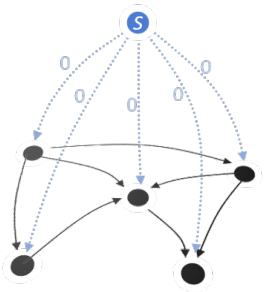
Given a directed graph where each edge is labelled with a weight, (i) if the graph contains no negative-weight cycles then for every pair of vertices compute the weight of the minimal-weight path between those vertices; (ii) if the graph contains a negative-weight cycle then detect that this is so.

IMPLEMENTATION AND ANALYSIS

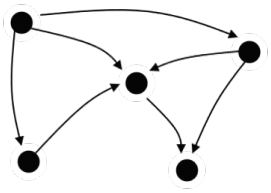
1. The helper graph. First build a helper graph, as shown below. Run Bellman-Ford on the helper graph, and let the minimum weight from s to v be d_v. (The direct path $s \to v$ has weight 0, so obviously $d_v \leq 0$. But if there are negative-weight edges in the graph, some vertices will have $d_v < 0$.) If Bellman-Ford reports a negative-weight cycle, then stop.



original graph, with edge weights $w(u \to v)$



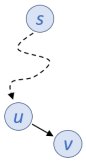
helper graph, with an extra vertex s and zero-weight edges $s \to v$ for all vertices v



a tweaked graph with modified edge weights $w'(u \to v)$

2. The tweaked graph. Define a tweaked graph which is like the original graph, but with different edge weights:

$$w'(u \to v) = d_u + w(u \to v) - d_v.$$



CLAIM: in this tweaked graph, every edge has $w'(u \to v) \geq 0$. PROOF: The relaxation equation, applied to the helper graph, says that $d_v \leq d_u + w(u \to v)$, therefore $w'(u \to v) \geq 0$.

3. Dijkstra on the tweaked graph. Run Dijkstra's algorithm V times on the tweaked graph, once from each vertex. (We've ensured that the tweaked graph has edge weights ≥ 0, so Dijkstra terminates correctly.) CLAIM: Minimum-weight paths in the tweaked graph are the same as in the original graph. PROOF: Pick any two vertices p and q, and any path between them

$$p = v_0 \to v_1 \to \cdots \to v_k = q.$$

What weight does this path have, in the tweaked graph and in the original graph?

This algebraic trick is called a *telescoping sum*.

$$\begin{aligned}
&\text{weight in tweaked graph} \\
&\quad = d_p + w(v_0 \to v_1) - d_{v_1} + d_{v_1} + w(v_1 \to v_2) - d_{v_2} + \cdots \\
&\quad = d_p + w(v_0 \to v_1) + w(v_1 \to v_2) + \cdots + w(v_{k-1} \to v_k) - d_q \\
&\quad = \text{weight in original graph} + d_p - d_q.
\end{aligned}$$

Since $d_p - d_q$ is the same for every path from p to q, the ranking of paths is the same in the tweaked graph as in the original graph (though of course the weights are different).

4. Wrap up. We've just shown that

$$\begin{array}{lcll}
\text{min weight} & & \text{min weight} & \\
\text{from } p \text{ to } q & = & \text{from } p \text{ to } q & - d_p + d_q \\
\text{in original graph} & & \text{in tweaked graph} &
\end{array}$$

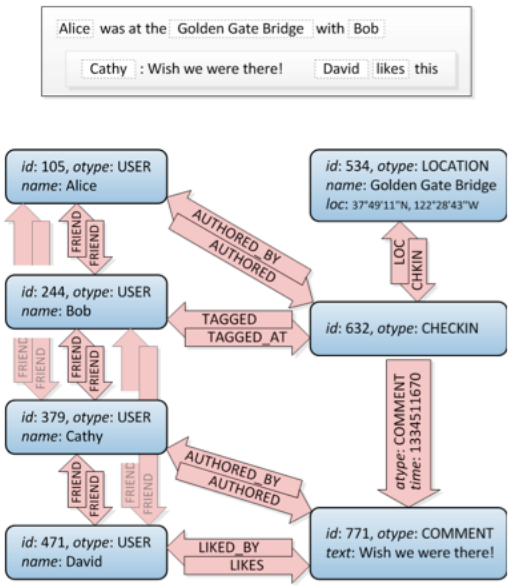
which solves the problem statement.

5.9. Graphs and big data*

This section of notes is not examinable.

FACEBOOK

Facebook sees the world as a graph of objects and associations, their *social graph*[6]:



Facebook represents this internally with classic database tables:

id	otype	attributes
105	USER	{name: Alice}
244	USER	{name: Bob}
379	USER	{name: Cathy}
471	USER	{name: David}
534	LOCATION	{name: Golden Gate Bridge, loc: (38.9,-77.04)}
632	CHECKIN	
771	COMMENT	{text: Wish we were there!}

from_id	to_id	edge_type
105	244	FRIEND
105	379	FRIEND
105	632	AUTHORED
244	105	FRIEND
244	379	FRIEND
244	632	TAGGED_AT

Why not use an adjacency list? Some possible reasons:

- Backups! Years of bitter experience have gone into today's databases, and they are very good and reliable for mundane tasks like backing up your data. The data is too big to fit in memory, and database tables are a straightforward way to store it on disk.
- Database tables can be indexed on many keys. If I have a query like "Find all edges to or from user 379 with timestamp no older than 24 hours", and if the edges table has indexes for columns from_id and to_id and timestamp, then the query can be answered quickly. In an adjacency list representation, we'd just have to trawl through all the edges.

[6] *TAO: Facebook's Distributed Data Store for the Social Graph*, Bronson et al., Usenix 2013

When you visit your home page, Facebook runs many queries on its social graph to populate the page. It needs to ensure that the common queries run very quickly, and so it has put considerable effort into indexing and caching.

Twitter also has a huge graph, with vertices for tweets and users, and edges for @mentions and follows. Like Facebook, it has optimized its graph database[7] to give rapid answers to 'broad but shallow' queries on the graph, such as "Who is following both the tweeter and the @mentioned user?"

GOOGLE MAPS

One of the jobs of a mapping platform is to find shortest paths (quickest, or fewest changes, or least walking, depending on the user's preferences). A popular platform like Google Maps has to answer a huge rate of such requests. One reaction is to use more efficient algorithms than Dijkstra's, such as the A^* algorithm which the final example sheet asks you to analyze. Another reaction is to precompute partial answers. Consider for example the road network. To travel any long distance, the only sensible route is to get on a motorway, travel along the motorway network, then get off the motorway. This suggests we might precompute all-to-all routes on the motorway network, and the shortest route between any location and its nearby motorway junctions, so that the final answer is a small lookup rather than a big computation. This is known as hierarchical routing.

Both A^* and hierarchical routing are optimizations that make sense when there are particular topological properties of the graph that we can make use of. The interplay between datasets (i.e. the characteristics of the graph) and algorithms is a fruitful topic of research.

GOOGLE, SPARK

Google first came to fame because they had a better search engine than anyone else. The key idea, by Brin and Page when they were PhD students at Stanford, was this: a webpage is likely to be 'good' if other 'good' webpages link to it. They built a search engine which ranked results not just by how well they matched the search terms, but also by the 'goodness' of the pages. They use the word PageRank rather than goodness, and the equation they used to define it is

$$\mathrm{PR}_v = \frac{1-\delta}{|V|} + \delta \sum_{u\,:\,u\to v} \frac{\mathrm{PR}_u}{|u.\mathsf{neighbours}|}$$

where $\delta = 0.85$ is put in as a 'dampening factor' that ensures the equations have a well-behaved unique solution.

How do we solve an equation like this, on a giant graph with one vertex for every webpage? Google said in 2013 that it indexes more than 30 trillion unique webpages, so the graph needs a cluster of machines to store it, and the computation has to be run on the cluster.

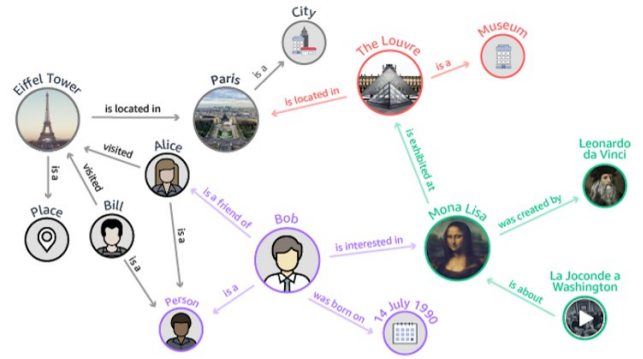
A popular platform for distributed computation (as of writing these notes in 2018) is called Spark[8]. It has a library that is tailor-made for distributed computation over graphs, and friendly tutorials.

KNOWLEDGE GRAPHS AND GRAPH DATABASES

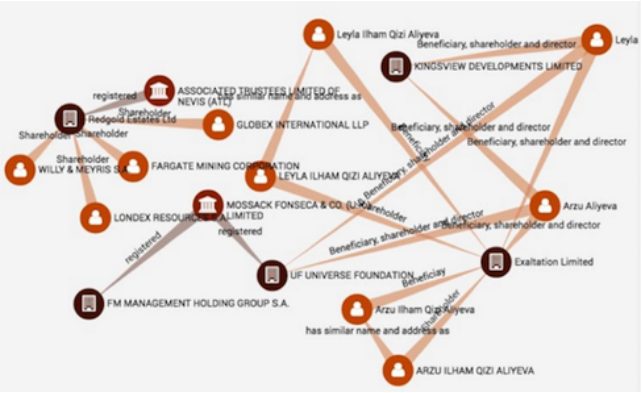
A knowledge graph is a graph designed to capture facts about real-world objects and their relationships.

[7] For a well written explanation of why and how they designed their graph database, `https://blog.twitter.com/engineering/en_us/a/2010/introducing-flockdb.html`

[8] `http://spark.apache.org/docs/latest/graphx-programming-guide.html#pagerank`



Knowledge graphs are used by Alexa and Google Assistant and so on, to hopefully be able to answer questions like "In what cities can I see art by Leonardo da Vinci?".



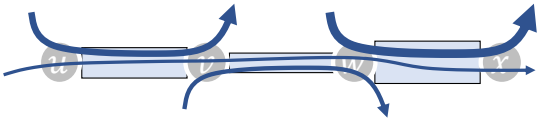
When the Panama Papers dataset was leaked[9], uncovering a complex network of offshore trusts, the journalists who got hold of it used a graph database called neo4j to help them understand it. You have learnt (or will learn) more about neo4j in IA/IB Databases.

[9] https://offshoreleaks.icij.org/pages/database

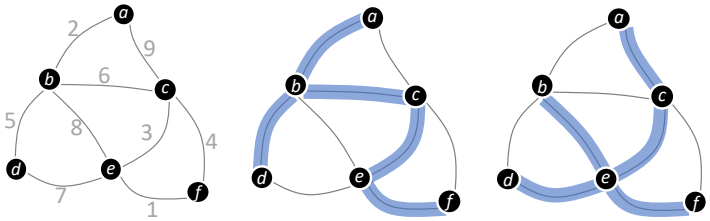
6. Flow and subgraph algorithms

In this section we will look at algorithms for finding structures within graphs. Here are two examples to illustrate the range of problems.

Example (Resource allocation in the Internet). Many problems in systems research boil down to resource allocation. Consider for example a graph in which each edge represents a link in the Internet, and has an associated bandwidth; in this picture the width of the edge measures its bandwidth, thus $v \leftrightarrow w$ has low bandwidth and $w \leftrightarrow x$ has high bandwidth. Suppose there are 4 TCP flows, each on its own route. Should each flow get equal throughput, even though one of the flows takes up three times as much resources as the others? Or should the goal be to maximize total throughput, which would result in the three-link flow getting nothing at all?



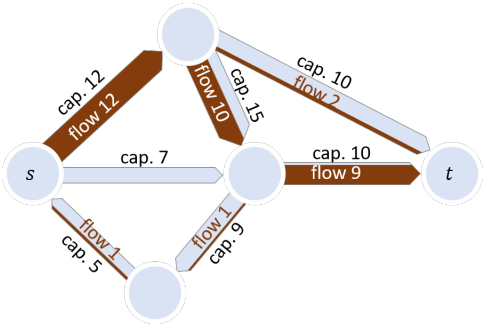
Example (Minimum spanning trees). Suppose we have to build a power grid to connect 6 cities. Given the costs of running cabling between locations, what is the cheapest power grid to build?



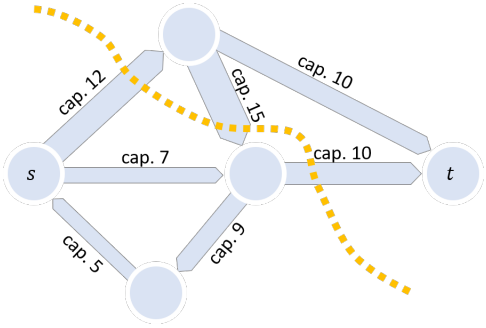
edge costs network of cost 17 network of cost 28

6.1. Max-flow min-cut theorem

For some applications, it's useful to consider a graph where each edge has a capacity. In the Internet each link has a maximum bandwidth it can carry; in the road network each road has a maximum amount of traffic it can handle; in an oil pipeline system each pipe has a capacity. Many interesting problems can be boiled down to the question: what is the maximum amount of stuff that can be carried between a given pair of vertices? First, some definitions.



A flow from s to t of value 11



A cut between s and t of capacity 22

DEFINITIONS

It's easy to generalise to multiple sources and sinks, rather harder to generalise to multiple types of stuff.

Consider a directed graph. Let each edge have a label $c(u \to v) > 0$ called the *capacity*. Let there be a *source vertex* s, and a *sink vertex* t. A *flow* is a set of edge labels $f(u \to v)$ such that

$$0 \le f(u \to v) \le c(u \to v) \quad \text{on every edge}$$

and

$$\sum_{u:\, u \to v} f(u \to v) = \sum_{w:\, v \to w} f(v \to w) \quad \text{at all vertices } v \in V \setminus \{s, t\}.$$

The second equation is called *flow conservation*, and it says that as much stuff comes in as goes out. The *value* of a flow is the net flow out of s,

$$\text{value}(f) = \sum_{u:\, s \to u} f(s \to u) - \sum_{u:\, u \to s} f(u \to s).$$

(It's easy to prove that the net flow out of s must be equal to the net flow into t. See Example Sheet 6.) A *cut* is a partition of the vertices into two sets, $V = S \cup \bar{S}$, with $s \in S$ and $t \in \bar{S}$. The *capacity* of a cut is

The capacity of the cut shown at the top of this page is indeed 22, not 37!

$$\text{capacity}(S, \bar{S}) = \sum_{\substack{u \in S,\ v \in \bar{S}: \\ u \to v}} c(u \to v).$$

In this section we will analyse the mathematical properties of flows and cuts. In Section 6.2 we will study an algorithm for computing flows.

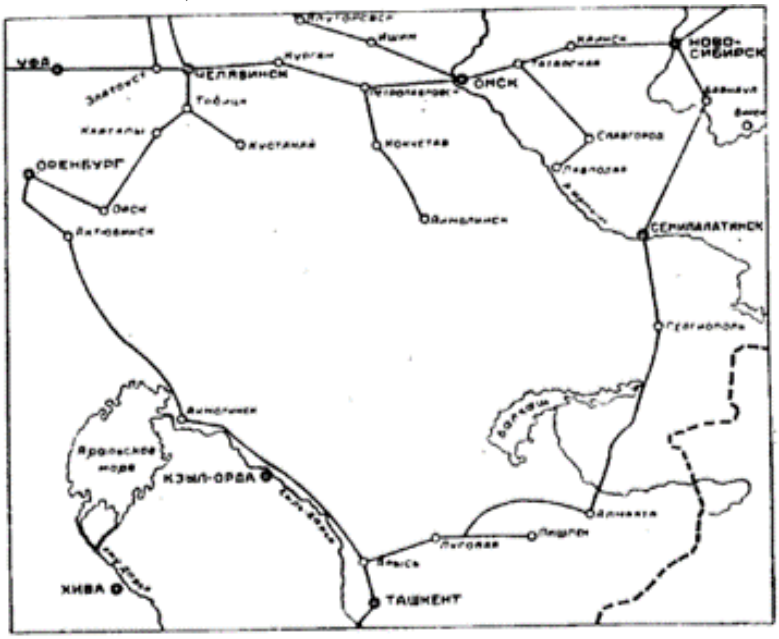
APPLICATION

Here is a pair of flow problems[10] that inspired the algorithm we'll describe shortly.

The Russian applied mathematician A.N.Tolstoy was the first to formalize the flow problem. He was interested in the problem of shipping cement, salt, etc. over the rail

[10] For further reading, see *On the history of the transportation and maximum flow problems* by Alexander Schrijver, `http://homepages.cwi.nl/~lex/files/histtrpclean.pdf`; and *Flows in railway optimization* by the same author, `http://homepages.cwi.nl/~lex/files/flows_in_ro.pdf`.

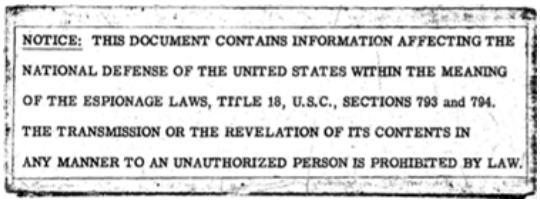
network. Formally, he posed the problem "Given a graph with edge capacities, and a list of source vertices and their supply capacities, and a list of destination vertices and their demands, find a flow that meets the demands."



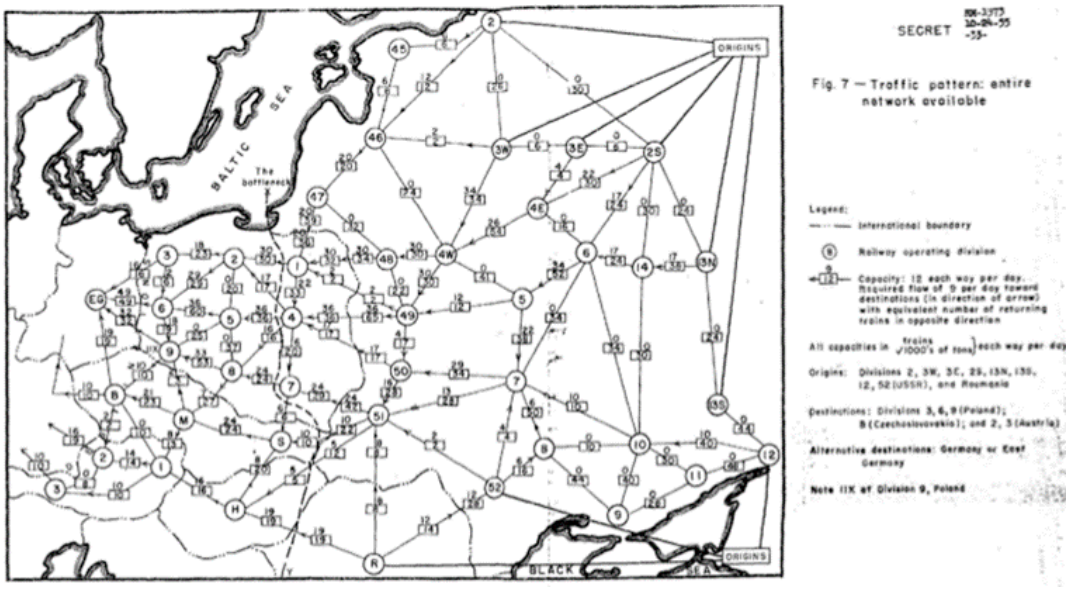
From *Methods of finding the minimum total kilometrage in cargo-transportation planning in space*, A.N.Tolstoy, 1930.

In this illustration, the circles mark sources and sinks for cargo, from Omsk in the north to Tashkent in the south.

The US military was also interested in flow networks during the cold war. If the Soviets were to attempt a land invasion of Western Europe through East Germany, they'd need to transport fuel to the front line. Given their rail network, and the locations and capacities of fuel refineries, how much could they transport? More importantly, which rail links should the US Air Force strike and how much would this impair the Soviet transport capacity?


NOTICE: THIS DOCUMENT CONTAINS INFORMATION AFFECTING THE NATIONAL DEFENSE OF THE UNITED STATES WITHIN THE MEANING OF THE ESPIONAGE LAWS, TITLE 18, U.S.C., SECTIONS 793 and 794. THE TRANSMISSION OR THE REVELATION OF ITS CONTENTS IN ANY MANNER TO AN UNAUTHORIZED PERSON IS PROHIBITED BY LAW.

From *Fundamentals of a method for evaluating rail net capacities*, T.E. Harris and F.S. Ross, 1955, a report by the RAND Corporation for the US Air Force (declassified by the Pentagon in 1999).



ANALYSIS

Theorem (Max-flow min-cut theorem). *For any flow f and any cut $(S, \bar{S})$,*

$$\text{value}(f) \leq \text{capacity}(S, \bar{S}).$$

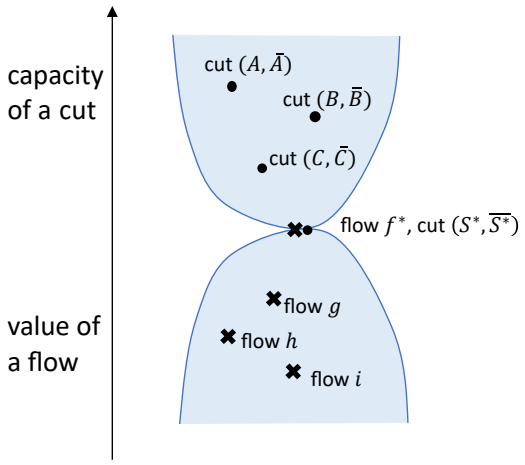
Proof. To simplify notation in this proof, we'll extend f and c to all pairs of vertices: if there is no edge $u \to v$, let $f(u \to v) = c(u \to v) = 0$.

$$\begin{aligned}
\text{value}(f) &= \sum_u f(s \to u) - \sum_u f(u \to s) && \text{by definition of flow value} \\
&= \sum_{v \in S} \left(\sum_u f(v \to u) - \sum_u f(u \to v) \right) && \text{by flow conservation} \\
&\qquad \text{(the term in brackets is zero for } v \neq s\text{)} \\
&= \sum_{v \in S} \sum_{u \in S} f(v \to u) + \sum_{v \in S} \sum_{u \notin S} f(v \to u) \\
&\quad - \sum_{v \in S} \sum_{u \in S} f(u \to v) - \sum_{v \in S} \sum_{u \notin S} f(u \to v) \\
&\qquad \text{(splitting the sum over } u \text{ into two sums, } u \in S \text{ and } u \notin S \text{)} \\
&= \sum_{v \in S} \sum_{u \notin S} f(v \to u) - \sum_{v \in S} \sum_{u \notin S} f(u \to v) && \text{by 'telescoping' the sum} \\
&\leq \sum_{v \in S} \sum_{u \notin S} f(v \to u) && \text{since } f \geq 0 \qquad (1) \\
&\leq \sum_{v \in S} \sum_{u \notin S} c(v \to u) && \text{since } f \leq c \qquad (2) \\
&= \text{capacity}(S, \bar{S}) && \text{by definition of cut capacity.}
\end{aligned}$$

This completes the proof. □

* * *

What's this theorem for? The theorem implies that if we're able to find a flow f^* and a matching cut $(S^*, \bar{S}^*)$ such that $\text{value}(f^*) = \text{capacity}(S^*, \bar{S}^*)$, then every other flow must have value $\leq \text{capacity}(S^*, \bar{S}^*)$, therefore f^* is the maximum possible flow. This suggests we design an algorithm that looks for both a flow and a cut; if it finds a matching pair then it's safe to terminate. The surprising thing is that it is indeed possible to find a matching pair ...



The objective "find a maximum flow" is a special case of a wider class of maximization problems known as *linear programming*. Many graph problems, including shortest path and minimum spanning trees, can be phrased as linear programming problems. For every problem in this class there is a systematic way to formulate a corresponding minimization problem, called the dual (in this case it is "find the minimum capacity cut"); and the solution to the original maximization problem matches the solution to the dual. What's more, there is a systematic way to construct an algorithm to solve them both, called primal-dual algorithms.

This brief outline hasn't explained *why* it's possible to find a matching flow and cut, but at least it tells you where to look—study optimization theory and linear algebra!

6.2. Ford-Fulkerson algorithm

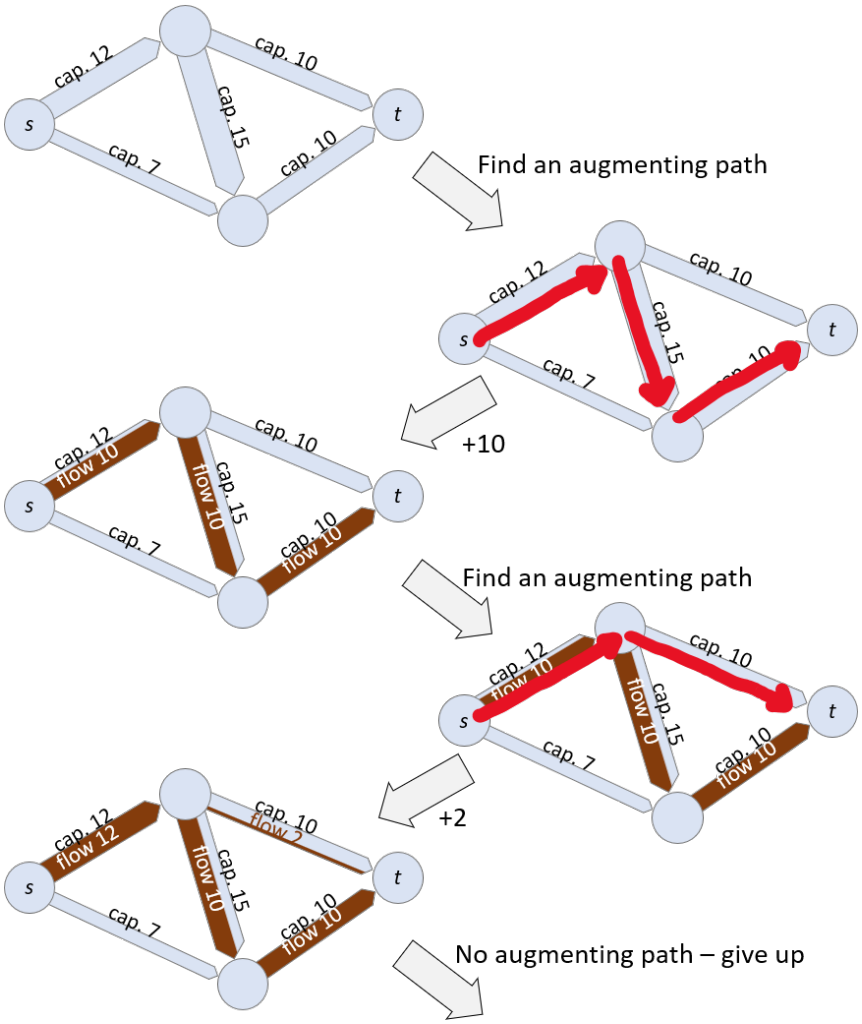
PROBLEM STATEMENT

Given a weighted directed graph g with a source s and a sink t, find a flow from s to t with maximum value (also called a *maximum flow*).

GENERAL IDEA

An obvious place to start is with a simple greedy algorithm: look for a path from s to t on which we can add flow, add as much as we can, and repeat. Because we're only adding flow along paths in the graph, we're guaranteed to end up with a valid flow, i.e. net flow in equals net flow out at every vertex apart from s and t.

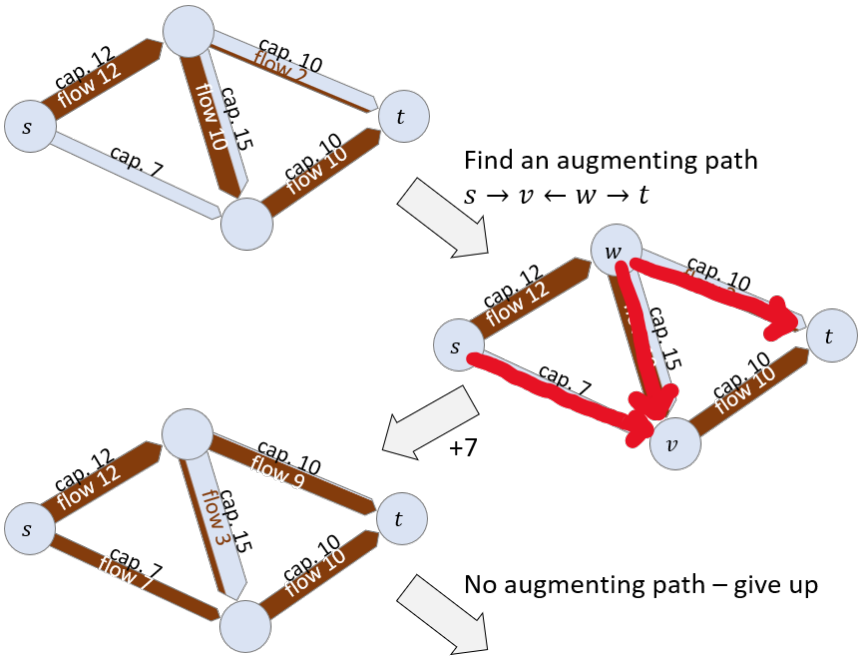
```
1  start with flow = 0
2  while True:
3      look for a path from s to t along which we can add some flow
4      (this is called the augmenting path)
5      if such a path exists:
6          add as much flow along it as we can
7      else:
8          break
```

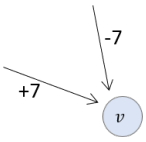


In this example, the greedy algorithm found a flow of size 12, then it finished. But we can easily see a flow of size 17 (10 on the top path, 7 on the bottom path). The naive greedy algorithm isn't good enough: it needs a way to undo its mistakes.

Here's a simple modification: change line 3 so that the augmenting path is allowed to contain both forwards and backwards arrows, for example $s \to v \leftarrow w \to t$. A forwards arrow like $s \to v$ means "we have room to increase $f(s \to v)$", and a backwards arrow like $v \leftarrow w$

means "we have room to decrease $f(w \to v)$". Line 6 should also be changed, to either add or decrease flow along the edges of the path, depending on their respective arrows.





It is important to understand why we're allowed to modify the flow along an augmenting path in this way. Formally, we need to explain why, after modifying the flow, it still satisfies flow conservation. To illustrate why this is true, consider for example vertex v: we're increasing $f(s \to v)$ by 7, and decreasing $f(w \to v)$ by 7, so the net flow at v is unchanged. Example sheet 6 asks you to work through the other cases.

We have proposed a simple greedy algorithm, and tweaked it to make a clever greedy algorithm. There are still questions to answer: (i) how do we actually search for the augmenting paths? (ii) how does the algorithm know when to stop, i.e. whether there is any augmenting path to find? (iii) why is this "clever greedy" strategy sufficient to get all the way to a maximum flow? The first two questions we'll address in the implementation, the last in the analysis and discussion.

IMPLEMENTATION

```
1  def ford_fulkerson(g, s, t):
2      # let f be a flow, initially empty
3      for u → v in g.edges:
4          f(u → v) = 0
5
6      # Define a helper function for finding an augmenting path
7      def find_augmenting_path():
8          # define a helper graph h on the same vertices as g
9          for each pair of vertices (v,w) in g:
10             if f(v → w) < c(v → w): give h an edge v → w with label "forwards"
11             if f(w → v) > 0: give h an edge v → w with label "backwards"
12         if h has a path from s to t:
13             return some such path, together with the labels of its edges
14         else:
15             # There is a set of vertices that we can reach starting from s;
16             # call this "the cut associated with flow f".
17             # We'll use this in the analysis.
18             return None
19
20     # Repeatedly find an augmenting path and add flow to it
21     while True:
```

```
22          p = find_augmenting_path()
23          if p is None:
24              break  # give up — can't find an augmenting path
25          else:
26              let the vertices of p be s = v_0, v_1, ..., v_k = t
27              δ = ∞ # amount by which we'll augment the flow
28              for each edge (v_i, v_{i+1}) along p:
29                  if the edge has label "forwards":
30                      δ = min(δ, c(v_i → v_{i+1}) − f(v_i → v_{i+1}))
31                  else the edge must have label "backwards":
32                      δ = min(δ, f(v_{i+1} → v_i))
33              # assert: δ > 0
34              for each edge (v_i, v_{i+1}) along p:
35                  if the edge has label "forwards":
36                      f(v_i → v_{i+1}) = f(v_i → v_{i+1}) + δ
37                  else the edge must have label "backwards":
38                      f(v_{i+1} → v_i) = f(v_{i+1} → v_i) − δ
39              # assert: f is still a flow (according to defn. in Section 6.1)
```

This pseudocode doesn't tell us how to choose the path in line 13. One sensible idea is 'pick the shortest path', and this version is called the Edmonds–Karp algorithm; it is a simple matter[11] of running breadth first search on the helper graph. Another sensible idea is 'pick the path that makes δ as large as possible', also due to Edmonds and Karp.

ANALYSIS OF RUNNING TIME

Be scared of the while loop in line 21: how can we be sure it will terminate? In fact, there are simple graphs with irrational capacities where the algorithm does *not* terminate. On the other hand,

Lemma. *If all capacities are integers then the algorithm terminates, and the resulting flow on each edge is an integer.*

Proof. Initially, the flow on each edge is 0, i.e. integer. At each execution of lines 27–32, we start with integer capacities and integer flow sizes, so we obtain δ an integer ≥ 0. It's not hard to prove the assertion on line 33, i.e. that $\delta > 0$, by thinking about the helper graph in find_augmenting_path. Therefore the total flow has increased by an integer after lines 34–38. The value of the flow can never exceed the sum of all capacities, so the algorithm must terminate. □

Now let's analyse running time, under the assumption that capacities are integer. We execute the while loop at most f^* times, where f^* is the value of maximum flow. We can build the helper graph and find a path in it using breadth first search, so find_augmenting_path is $O(V+E)$. Lines 27–38 involve some operations per edge of the augmenting path, which is $O(V)$ since the path is of length $\leq V$. Thus the total running time is $O\big((E+V)f^*\big)$. There's no point including the vertices that can't be reached from s, so we might as well assume that all vertices can be reached from s, so $E \geq V-1$ and the running time can be written $O(Ef^*)$.

It is worth noting that the running time we found depends on the values in the input data (via f^*) rather than just the size of the data. On one hand this is good because any analysis that ignores the data can't be very informative. On the other had it's bad because we don't have a useful upper bound for f^*. This is a common feature of many optimization algorithms, and of machine learning algorithms.

The Edmonds–Karp version of the algorithm can be shown to have running time $O(E^2V)$.

[11] Be careful when implementing your breadth first search, because the helper graph could have two edges in the same direction between a pair of nodes.

ANALYSIS OF CORRECTNESS

The assertion on line 39, namely that the algorithm does indeed produce a flow, is an exercise on Example Sheet 6. What about the main goal of the problem statement — does the algorithm produce a maximum flow?

Theorem. *Suppose the algorithm terminates, and f^* is the final flow it produces. Let S^* be the cut associated with flow f^*, from line 16 in the final call to* `find_augmenting_path()`*. Then*

1. *the value of f^* is equal to the capacity of the cut $(S^*, \bar{S}^*)$, and*
2. *f^* is a maximum flow.*

Proof (of 1). By the condition on line 11, $f^*(w \to v) = 0$ for all $v \in S^*$, $w \notin S^*$, so inequality (1) on page 28 is an equality. By the condition on line 10, $f^*(v \to w) = c(v \to w)$ for all $v \in S^*$, $w \notin S^*$, so inequality (2) is also an equality. Thus, value(f^*) is equal to capacity$(S^*, \bar{S}^*)$.

Proof (of 2). Recall the Max-Flow Min-Cut theorem from Section 6.1. It says that for *any* flow f and any cut $(S, \bar{S})$,

$$\text{value}(f) \leq \text{capacity}(S, \bar{S}).$$

Therefore, setting S to be the final cut S^* and taking the maximum over all possible flows f,

$$\max_{\text{all flows } f} \text{value}(f) \leq \text{capacity}(S^*, \bar{S}^*).$$

But by part 1 this bound is achieved by flow f^*. Therefore f^* is a maximum flow. □

A cut corresponding to a maximum flow is called a *bottleneck cut*. (The bottleneck cut might not be unique, and the maximum flow might not be unique either, but the maximum flow *value* and bottleneck cut *capacity* are unique.) The RAND report shows a bottleneck cut, and suggests it's the natural target for an air strike.

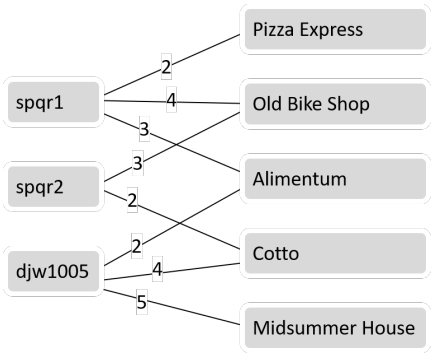
6.3. Matchings

There are several graph problems that don't on the surface look like flow networks, but which can be solved by translating them into a well-chosen maximum flow problem. Here's an example. Example Sheet 6 has more.

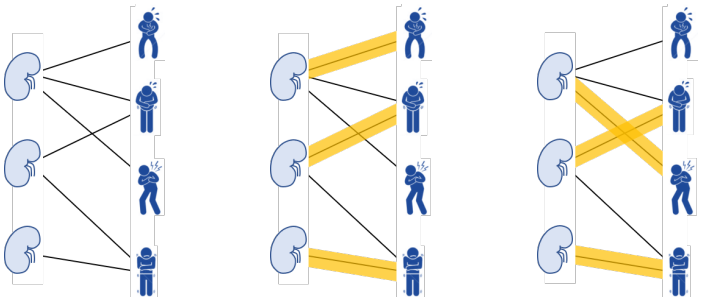
* * *

A *bipartite graph* is one in which the vertices are split into two sets, and all the edges have one end in one set and the other end in the other set. We'll assume the graph is undirected. For example

- Vertices for medical school graduates, vertices for hospitals offering residency training, and edges for each application the medic has made to a hospital.
- Vertices for Yelp users, vertices for restaurants, and edges labelled with weights to indicate the user's rating of the restaurant.

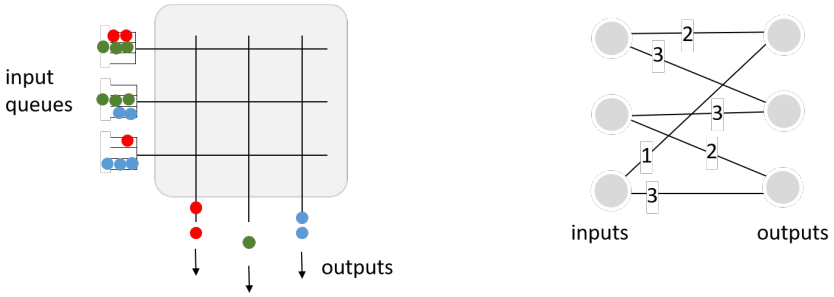


A *matching* in a bipartite graph is a selection of some or all of graph's edges, such that no vertex is connected to more than one edge in this selection. For example, kidney transplant donors and recipients, with edges to indicate compatibility. The *size* of a matching is the number of edges it contains. A *maximum matching* is one with the largest possible size. There may be several maximum matchings.



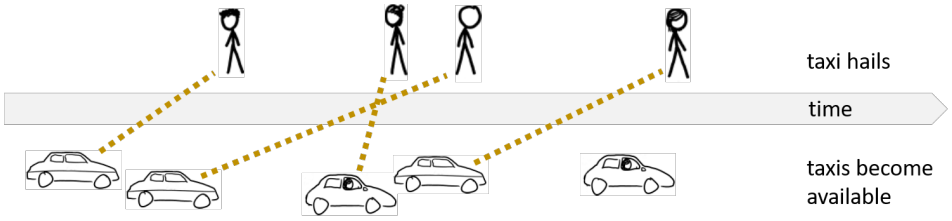
FURTHER APPLICATIONS

Example (Internet switches). The silicon in the heart of an Internet router has the job of forwarding packets from inputs to outputs. Every clock tick, it can take at most one packet from each input, and it can send at most one packet to each output—in other words, it selects a matching from inputs to outputs. It turns out to be useful to weight the edges by the number of packets waiting to be sent, and to pick a matching with the highest possible total weight.



Example (Taxi scheduling). A company like Uber has to match taxis to passengers. When there are passengers who have made requests, which taxis should they get[12]? This is an example of an *online matching problem*. (As opposed to the offline matching problem, in which all the vertices and edges are known in advance.) In online problems, bad choices will have kock-on effects.

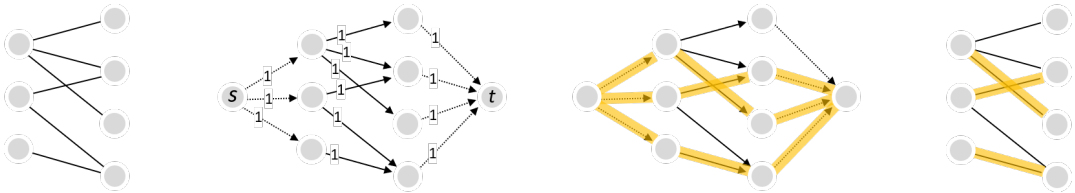
The simple greedy strategy "pick the nearest available taxi as soon as a request is made" might lead to shortages on the perimeter of the network, or to imbalanced workloads among drivers. We could turn it into an offline problem by batching, for example "once a minute, put edges from each waiting passenger to the ten nearest available vehicles, and look for a maximum matching".



PROBLEM STATEMENT AND IMPLEMENTATION

How can we find a maximum matching in a bipartite graph? Let's translate the matching problem into a flow problem, as follows.

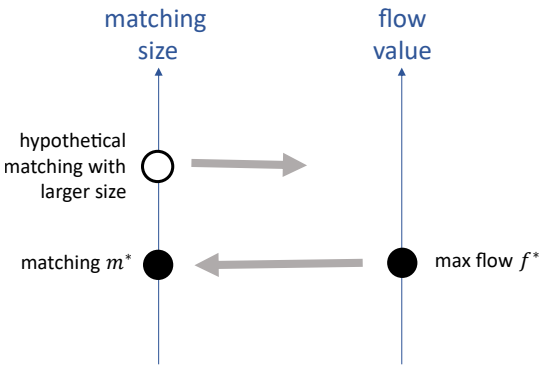
1. start with a bipartite graph
2. create a helper graph as follows: add a source s with edges to each left-hand vertex; add a sink with edges from each right-hand vertex; turn the original edges into directed edges from left to right; give all edges capacity 1
3. run the Ford-Fulkerson algorithm on the helper graph to find a maximum flow from s to t
4. interpret that flow as a matching in the original bipartite graph



ANALYSIS

It's easy to not even notice that there's something that needs to be proved here. It's actually a rather subtle argument. We need a proof that translates in two directions:

[12] Figure elements from Randall Munroe, `https://what-if.xkcd.com/9/` and `https://what-if.xkcd.com/93/`



1. The maximum flow f^* in the helper graph has to translate back into a matching, call it m^*. *What could go wrong? The maximum flow might have fractional flow on some edges, which would mean it can't be translated into a matching.*
2. Hypothetically, if there were a matching of size larger than m^*, then it must translate into a flow with value larger than value(f^*). But such a flow can't exist, therefore such a matching can't exist either. *What could go wrong? We might have a dodgy translation where some matchings can't be translated into flows, or where larger size matchings translate into smaller value flows.*

Once we figure out what we have to prove, the proof is easy.

Theorem. *1. Step 3 of the algorithm described above terminates, and the flow f^* that it produces can be translated into a matching m^*, with* $\text{size}(m^*) = \text{value}(f^*)$.

2. Any matching m translates into a flow f with $\text{size}(m) = \text{value}(f)$. *In particular, if there were any matching larger than m^* then the corresponding flow would have value larger than that of f^*.*

Hence m^* is a maximum matching.

Proof (of 1). The lemma in Section 6.2 on page 31 tells us that the Ford-Fulkerson algorithm terminates, since all edge capacities are integer. Write f^* for the flow produced by Ford-Fulkerson. The lemma tells us furthermore that f^* is integer on all edges. Since the edge capacities are all 1, the flow must be 0 or 1 on all edges. Translate f^* into a matching m^*, by simply selecting all the edges in the original bipartite graph that got $f^* = 1$. The capacity constraints on edges from s means that each left-hand vertex has either 0 or 1 flow coming in, so it must have 0 or 1 flow going out, therefore it is connected to at most one edge in m^*. Similarly, each right-hand vertex is connected to at most one edge in m^*. Therefore m^* is a matching.

Proof (of 2). Take any matching m and translate it into a flow f in the natural way, i.e. with a flow of 1 from s to every matched left hand vertex, and similarly for t. From this translation it's obvious that

$$\text{size}(m) = \text{value}(f).$$

Proof (of theorem). If m^* were not a maximum size matching then there must be a larger matching m'. By part 2 it translates into a flow f' with

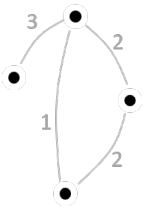
$$\text{size}(m') > \text{size}(m^*) \qquad \Longrightarrow \qquad \text{value}(f') > \text{value}(f^*).$$

But this contradicts the choice of f^* to be a maximum flow. Hence the premise is false, i.e. m^* is a maximum size matching. □

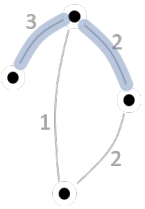
6.4. Prim's algorithm

See Section 5.1 for the definition of 'connect' and 'tree'.

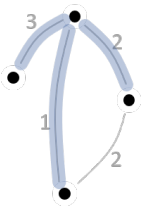
Given a connected undirected graph with edge weights, a *minimum spanning tree* (MST) is a tree that 'spans' the graph i.e. connects all the vertices, and which has minimum weight among all spanning trees. (The *weight* of a tree is just the sum of the weights of its edges.)



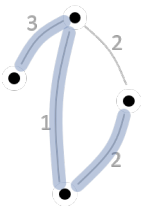
undirected graph with edge weights



a tree, but not spanning



spanning tree of weight 6



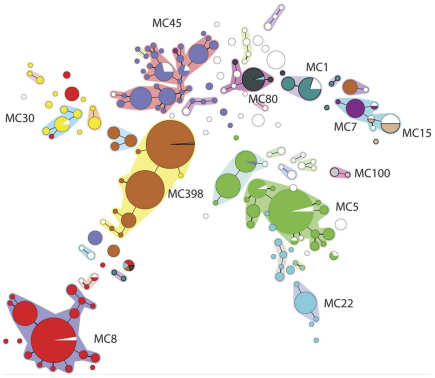
spanning tree of weight 6

APPLICATIONS

- The MST problem was first posed and solved by the Czech mathematician Borůvka in 1926, motivated by a network planning problem. His friend, an employee of the West Moravian Powerplants company, put to him the question: if you have to build an electrical power grid to connect a given set of locations, and you know the costs of running cabling between locations, what is the cheapest power grid to build?

The 'edit distance' between two strings is a measure of how different they are. See Section 1.2.

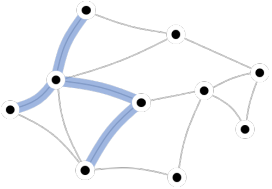
- Minimal spanning trees are a useful tool for exploratory data analysis. In this illustration from bioinformatics[13], each vertex is a genotype of *Staphylococcus aureus*, and the size shows the prevalance of that genotype in the study sample. Let the there be edges between all genotypes, weighted according to edit distance. The illustration shows the MST, after some additional high-weight edges are removed.



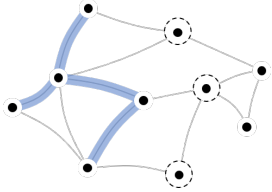
GENERAL IDEA

We'll build up the MST greedily. Suppose we've already built a tree containing some of the vertices (start it with just a single vertex, chosen arbitrarily). Look at all the edges between the tree we've built so far and the adjacent vertices that aren't part of the tree, pick the edge of lowest weight among these and add it to the tree, then repeat.

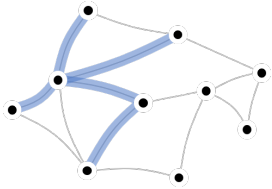
This greedy algorithm will certainly give us a spanning tree. To prove that it's a MST takes some more thought.



a tree build up with four edges so far



three candidate vertices to add next



pick the cheapest of the four connecting edges and add it to the tree

[13] From *Multiple-Locus Variable Number Tandem Repeat Analysis of Staphylococcus Aureus*, Schouls et al., PLoS ONE 2009.

PROBLEM STATEMENT

Given a connected undirected graph with edge weights, construct an MST.

IMPLEMENTATION

We don't need to recompute the nearby vertices every iteration. Instead we can use a structure very similar to Dijkstra's algorithm for shortest paths: store a 'frontier' of vertices that are neighbours of the tree, and update it each iteration. This algorithm is due to Jarnik (1930), and independently to Prim (1957) and Dijkstra (1959). When the algorithm terminates, an MST is formed from the edges

$$\{v \leftrightarrow v.\text{come\_from} \ : \ v \in V, v \neq s\}.$$

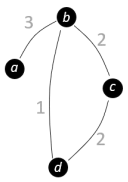
Compared to Dijkstra's algorithm, we need some extra lines to keep track of the tree (lines labelled +), and two modified lines (labelled ×) because here we're interested in 'distance from the tree' whereas Dijkstra is interested in 'distance from the start node'. The start vertex s can be chosen arbitrarily.

```
1   def prim(g, s):
2       for v in g.vertices:
3           v.distance = ∞
4 +         v.in_tree = False
5 +     s.come_from = None
6       s.distance = 0
7       toexplore = PriorityQueue([s], lambda v : v.distance)
8
9       while not toexplore.isempty():
10          v = toexplore.popmin()
11 +        v.in_tree = True
12          # Let t be the graph made of vertices with in_tree=True,
13          # and edges {w—w.come_from, for w in g.vertices excluding s}.
14          # Assert: t is part of an MST for g
15          for (w, edgeweight) in v.neighbours:
16 ×            if (not w.in_tree) and edgeweight < w.distance:
17 ×                w.distance = edgeweight
18 +                w.come_from = v
19                  if w in toexplore:
20                      toexplore.decreasekey(w)
21                  else:
22                      toexplore.push(w)
```

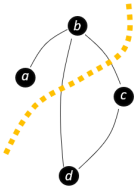
ANALYSIS

Running time. It's easy to check that Prim's algorithm terminates. It is nearly identical to Dijkstra's algorithm, and exactly the same analysis of running time applies: is $O(E+V \log V)$, assuming the priority queue is implemented using a Fibonacci heap.

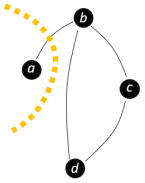
Correctness. **The proof of correctness is not examinable. It is all maths, no algorithm.** To prove that Prim's algorithm does indeed find an MST (and for many other problems to do with constructing networks on top of graphs) it's helpful to make a definition. A *cut* of a graph is an assignment of its vertices into two non-empty sets, and an edge is said to *cross* the cut if its two ends are in different sets.



an undirected graph with edge weights



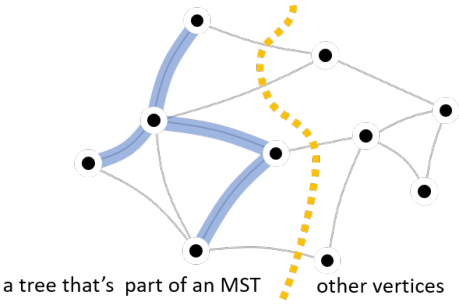
a cut into $\{a, b\}$ and $\{c, d\}$, with two edges crossing the cut



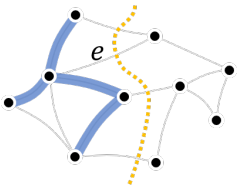
a cut into $\{a\}$ and $\{b, c, d\}$, with one edge crossing the cut

Prim's algorithm builds up a tree, adding edges greedily. By the following theorem, Prim's algorithm produces an MST.

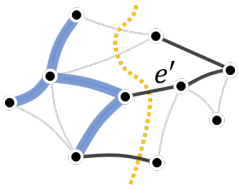
Theorem. *Suppose we have a forest F and a cut C such that (i) C contains no edges of F, and (ii) there exists a MST containing F. If we add to F a min-weight edge in C, then the result is still part of a MST.*



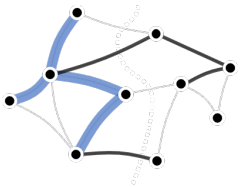
Proof. Let F be the forest, and let $\bar{F}$ be an MST that F is part of (the condition of the theorem requires that such an $\bar{F}$ exists). Let e be the a minimum weight edge across the cut. We want to show that there is an MST that includes $F \cup \{e\}$. If $\bar{F}$ includes edge e, we are done.



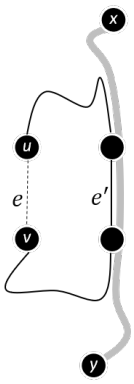
the forest F



a MST $\bar{F}$



a different MST $\hat{F}$



Suppose then that $\bar{F}$ doesn't contain e. Let u and v be the vertices at either end of e, and consider the path in $\bar{F}$ between u and v. (There must be such a path, since $\bar{F}$ is a spanning tree, i.e. it connects all the vertices.) This path must cross the cut (since its ends are on different sides of the cut). Let e' be an edge in the path that crosses the cut. Now, let $\hat{F}$ be like $\bar{F}$ but with e added and e' removed.

It's easy to see that weight$(\hat{F}) \leq$ weight$(\bar{F})$: e is a min-weight edge in the cut, so weight$(e) \leq$ weight(e'). CLAIM: $\hat{F}$ is connected. If this claim is true, then $\hat{F}$ must be a tree, since it has the same number of edges as $\bar{F}$ namely $|V| - 1$. Therefore it is a MST including $F \cup \{e\}$, and the theorem is proved.

PROOF OF CLAIM. Pick any two vertices x and y. Since $\bar{F}$ is a spanning tree, there is a path in $\bar{F}$ from x to y. If this path doesn't use e' then it is a path in $\hat{F}$, and we are done. If it does use e', consider the paths $x - y$ and $u - v$ in $\bar{F}$, both of which use e'. Either x and u are on one side of e' and y and v are on the other (as illustrated), or vice versa. Either way, we can build a path $x - y$ using e instead of e', by splicing in the relevant part of the $u - v$ path. This new path we've built is in $\hat{F}$. Since $\hat{F}$ contains a path between any two vertices x and y, it is connected. □

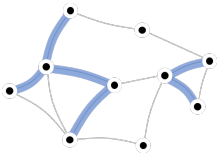
6.5. Kruskal's algorithm

Another algorithm for finding a minimum spanning tree is due to Kruskal (1956). It makes the same assumptions as Prim's algorithm. Its running time is worse. It does however produce intermediate states which can be useful.

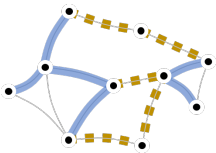
GENERAL IDEA

Kruskal's algorithm builds up the MST by agglomerating smaller subtrees together. At each stage, we've built up some fragments of the MST. The algorithm greedily chooses two fragments to join together, by picking the lowest-weight edge that will join two fragments.

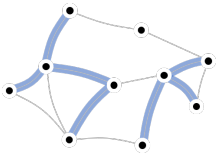
Kruskal's algorithm maintains a 'forest'. Look back at Section 5.1 for the definition.



four tree fragments have been found so far, including two trees that each consist of a single vertex



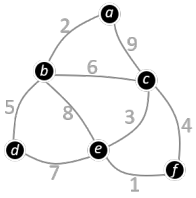
five candidate edges that would join two fragments



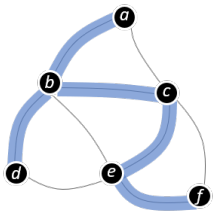
pick the cheapest of the five candidate edges, and add it, thereby joining two fragments

APPLICATION

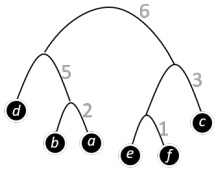
If we draw the tree fragments another way, the operation of Kruskal's algorithm looks like clustering, and its intermediate stages correspond to a classication tree:



an undirected graph with edge weights

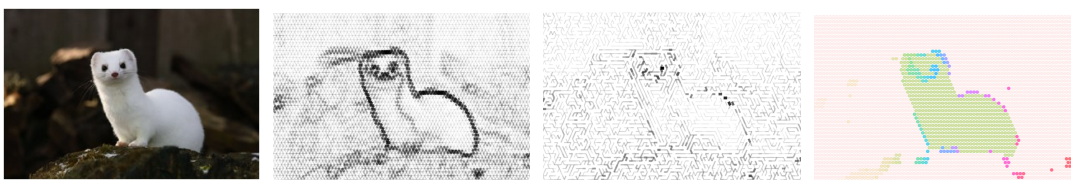


the MST found by Kruskal's algorithm



draw each fragment as a subtree, and draw arcs when two fragments are joined

This can be used for image segmentation. Here we've started with an image, put vertices on a hexagonal grid, added edges between adjacent vertices, given low weight to edges where the vertices have similar colour and brightness, run Kruskal's algorithm to find an MST, split the tree into clusters by removing a few of the final edges, and coloured vertices by which cluster they belong to.



PROBLEM STATEMENT

(Same as for Prim's algorithm.) Given a connected undirected graph with edge weights, construct an MST.

IMPLEMENTATION

This code uses a data structure called a DisjointSet. This is used to keep track of a collection of disjoint sets (sets with no common elements), also known as a partition. We'll learn more about it in Section 7.4. Here, we're using it to keep track of which vertices are in which fragment. Initially (lines 4–5) every vertex is in its own fragment. As the algorithm proceeds, it considers each edge in turn, and looks up the vertex-sets containing the start and the end of the edge. If they correspond to different fragments, it's safe to join the fragments, i.e. merge the two sets (line 13).

Lines 6 and 8 are used to iterate through all the edges in the graph in order of edge weight, lowest edge weight first.

```
1  def kruskal(g):
2      tree_edges = []
3      partition = DisjointSet()
4      for v in g.vertices:
5          partition.addsingleton(v)
6      edges = sorted(g.edges, sortkey = lambda u,v,edgeweight: edgeweight)
7
8      for (u,v,edgeweight) in edges:
9          p = partition.getsetwith(u)
10         q = partition.getsetwith(v)
11         if p != q:
12             tree_edges.append((u,v))
13             partition.merge(p, q)
14             # Let f be the forest made up of edges in tree_edges.
15             # Assert: f is part of an MST
16             # Assert: f has one connected component per set in partition
17
18     return tree_edges
```

ANALYSIS

Running time. The running time of Kruskal's algorithm depends on how DisjointSet is implemented. We'll see in Section 7.4 that all the operations on DisjointSet can be done in $O(1)$ time[14]. The total cost is $O(E \log E)$ for the sort on line 6; $O(E)$ for iterating over edges in lines 8–11; and $O(V)$ for lines 12–13, since there can be at most V merges. So the total running time is $O(E \log E)$.

The maximum possible number of edges in an undirected graph is $V(V-1)/2$, and the minimum number of edges in a connected graph is $V - 1$, so $\log E = \Theta(\log V)$, and so the running time can be written $O(E \log V)$.

Correctness. To prove that Kruskal's algorithm finds an MST, we apply the theorem used for the proof of Prim's algorithm, as follows. When the algorithm merges fragments p and q, consider the cut of all vertices into p versus not-p; the algorithm picks a minimum-weight edge across this cut, and so by the theorem we've still got an MST.

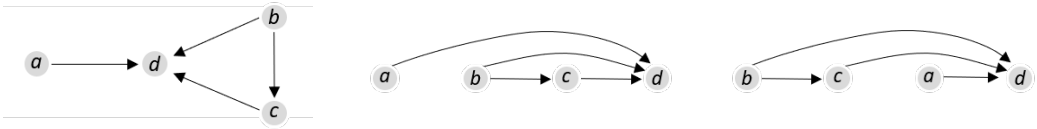
[14] This is a white lie. The actual complexity is $O(\alpha_n)$ for a DisjointSet with n elements, where α_n is a function that grows extraordinarily slowly.

6.6. Topological sort

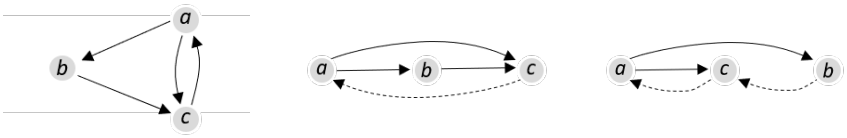
A directed graph can be used to represent ordering or preferences. We might then like to find a *total ordering* (also known as a *linear ordering* or *complete ranking*) that's compatible.

This problem is in the same general category as finding a minimal spanning tree: they are all problems of discovering organisation within a graph.

Here's a simple graph and two possible total orderings.



Does there exist a total order? If the graph has cycles, then no.

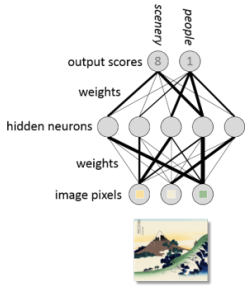


Recall the definition of a *directed acyclic graph* (DAG). A *cycle* is a path from a vertex back to itself, following the edge directions, and a directed graph is called *acyclic* if it has no cycles. We will see that, in a DAG, a total ordering can always be found.

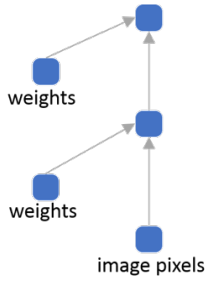
Don't get muddled by the word 'acyclic'. A DAG doesn't have to be a tree, and it might have multiple paths between vertices. The top row of graphs on this page are all DAGs.

APPLICATIONS

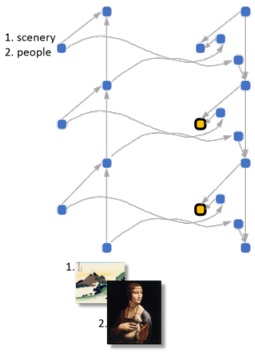
- Deep learning systems like TensorFlow involve writing out the learning task as a collection of computational steps, each of which depends on the answers of some of the preceding steps. Write $v_1 \to v_2$ to mean "Step v_2 depends on the output of v_1." If the computation graph is a DAG, then we can find an order in which to run all the computational steps. If it's not a DAG, then there is a circular dependency.



an image classifier, implemented with a deep neural network; the magic is finding good link weights

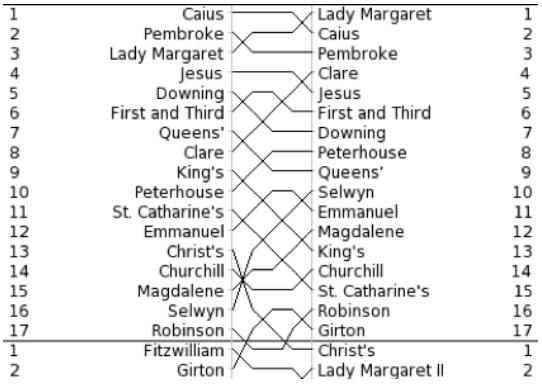


a DAG computational graph depicting how the classifier operates



a DAG computational graph for computing how the weights should be updated, based on a training dataset of pre-labelled images

- The river Cam isn't wide enough for a conventional race between all the rowing boats that want to compete. Instead, the Bumps evolved, as a way of ranking boats based on pairwise comparisons. The competition takes place over four days. On the first day, the boats start out spaced evenly along a stretch of the river, in order of last year's ranking. They start rowing all at the same time, and each boat tries to catch up—bump—the boat ahead. If this happens, then both boats move to the side of the river and withdraw from this day's race, and they switch their starting positions for the next day's race. Four days of the Bumps give us a set of pairwise comparisons: if boat v_1 bumps v_2, then we know v_1 is faster than v_2. Here are the men's bumps from May 2016. What are the total orderings consistent with this data, if any?



If the pairwise comparisons don't form a DAG, then it's impossible to find a total order—but we can still look for a order that's mostly consistent. There are many applications in machine learning with this flavour, where we think there is some hidden order or structure which we have to reconstruct based on noisy data.

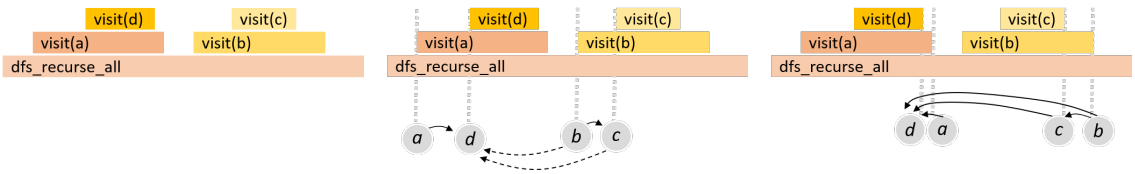
GENERAL IDEA

Recall depth-first search. After reaching a vertex v, it visits all v's children and other descendants. We want v to appear earlier in the ordering than all its descendants. So, can we use depth-first search to find a total ordering?

Here again is the depth-first search algorithm. This is dfs_recurse from Section 5.2, but modified so that it visits the entire graph (rather than just the part reachable from some given start vertex).

```
def dfs_recurse_all(g):
    for v in g.vertices:
        v.visited = False
    for v in g.vertices:
        if not v.visited:
            visit(v)  # start dfs from v

def visit(v):
    v.visited = True
    for w in v.neighbours:
        if not w.visited:
            visit(w)
```

A standard way to visualise program execution is with a *flame chart*. Time goes on the horizontal axis, each function call is shown as a rectangle, and if function f calls function g then g is drawn above f. Here is a flame chart for the graph at the beginning of this section.



If we order vertices by when the algorithm first visits them, it turns out not to be a total order. A better guess is to order vertices by when visit(v) *returns*.

PROBLEM STATEMENT

Given a directed acyclic graph (DAG), return a total ordering of all its vertices, such that if $v_1 \to v_2$ then v_1 appears before v_2 in the total order.

ALGORITHM

This algorithm is due to Knuth. It is based on dfs_recurse_all, with some extra lines (labelled +). These extra lines build up a linked list for the rankings, as the algorithm visits and leaves each vertex.

```
1  def toposort(g):
2      for v in g.vertices:
3          v.visited = False
4          # v.colour = 'white'
5  +   totalorder = []  # an empty list
6      for v in g.vertices:
7          if not v.visited:
8              visit(v, totalorder)
9  +   return totalorder
10
11 def visit(v, totalorder):
12     v.visited = True
13     # v.colour = 'grey'
14     for w in v.neighbours:
15         if not w.visited:
16             visit(w, totalorder)
17 +   totalorder.prepend(v)
18     # v.colour = 'black'
```

This listing also has some commented lines which aren't part of the algorithm itself, but which are helpful for arguing that the algorithm is correct. They're a bit like assert statements: they're there for our understanding of the algorithm, not for its execution.

ANALYSIS

Running time. We haven't changed anything substantial from dfs_recurse so the analysis in Section 5.2 still applies: the running time is $O(V + E)$.

Theorem (Correctness). *The toposort algorithm terminates and returns totalorder which solves the problem statement.*

Proof. Pick any edge $v_1 \to v_2$. We want to show that v_1 appears before v_2 in totalorder. It's easy to see that every vertex is visited exactly once, and on that visit (1) it's coloured grey, (2) some stuff happens, (3) it's coloured black. Let's consider the instant when v_1 is coloured grey. At this instant, there are three possibilities for v_2:

- v_2 is black. If this is so, then v_2 has already been prepended to the list, so v_1 will be prepended after v_2, so v_1 appears before v_2.
- v_2 is white. If this is so, then v_2 hasn't yet been visited, therefore we'll call visit(v_2) at some point during the execution of lines 14–16 in visit(v_1). This call to visit(v_2) must finish before returning to the execution of visit(v_1), so v_2 gets prepended earlier and v_1 gets prepended later, so v_1 appears before v_2.
- v_2 is grey. If this is so, then there was an earlier call to visit(v_2) which we're currently inside. The call stack corresponds to a path in the graph from v_2 to v_1. But we've picked an edge $v_1 \to v_2$, so there is a cycle, which is impossible in a DAG. This is a contradiction, so it's impossible that v_2 is grey. □

* * *

The breakpoint proof technique. The proof technique we used here was (1) consider an instant in time at which the algorithm has just reached a line of code; (2) reason about the current

state of all the variables, and the call stack, using mathematical logic. This is the same structure as the proof of correctness of Dijkstra's algorithm.

For this proof technique to work, we may need to store extra information about program state, so that the mathematical reasoning can use it. In this case, we invented the variable v.colour, which records a useful fact about what happened in the past. The algorithm doesn't need it, but it's useful for the maths proof.