

Algorithms

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1 Complexity

A course on the study of algorithms.

Definition 1.1 (Algorithm)

An **algorithm** is a procedure for solving a mathematical problem in a *finite* number of steps. It should be

1. finite,
2. correct,
3. efficient

An algorithm, with respect to some inputs \mathbf{n} , will have a runtime that is some function f . We would like a formal way to analyze the asymptotic behavior between two functions.

Definition 1.2 (Complexity)

Given two positive functions f, g ,

1. $f = O(g)$ if f/g is bounded.^a
2. $f = \Omega(g)$ if g/f is bounded, i.e. $g = O(f)$.
3. $f = \Theta(g)$ if $f = O(g)$ and $g = O(f)$.

There are two notions of complexity here. We can compare f and g with respect to the *value* N of the input, or we can compare them with respect to the *number of bits* n in the input. While we mostly use the complexity w.r.t. the value, we should be aware for certain (especially low-level operations), the bit complexity is also important.

Let's do a quick comparison of various functions. Essentially, if we want to figure out the complexity of two positive functions f, g ,¹ we can simply take the limit.

$$\lim_{x \rightarrow +\infty} \frac{f(x)}{g(x)} = \begin{cases} 0 & \implies f = O(g) \\ 0 < x < +\infty & \implies f = \Theta(g) \\ +\infty & \implies f = \Omega(g) \end{cases} \quad (1)$$

Most of the time, we will have to use L'Hopital's rule to derive these actual limits, but the general trend is

1. $\log n$ is small
2. $\text{poly}(n)$ grows faster
3. $\exp(n)$ grows even faster
4. $n!$ even faster
5. n^n even faster

Theorem 1.1 (Properties)

Some basic properties, which shows very similar properties to a vector space.

1. Transitivity.

$$f = O(g), g = O(h) \implies f = O(h) \quad (2)$$

$$f = \Omega(g), g = \Omega(h) \implies f = \Omega(h) \quad (3)$$

$$f = \Theta(g), g = \Theta(h) \implies f = \Theta(h) \quad (4)$$

$$(5)$$

^aNote that it is more accurate to write $f \in O(g)$, since we consider $O(g)$ a class of functions for which the property holds.

¹These will be positive since the runtime must be positive.

2. Linearity.

$$f = O(h), g = O(h) \implies f + g = O(h) \quad (6)$$

$$f = \Omega(h), g = \Omega(h) \implies f + g = \Omega(h) \quad (7)$$

$$f = \Theta(h), g = \Theta(h) \implies f + g = \Theta(h) \quad (8)$$

$$(9)$$

Example 1.1 ()

Compare the following functions.

1. $f(n) = \log_{10}(n), g(n) = \log_2(n)$. Since they are different bases, we can write $f(n) = \log(n)/\log(10)$ and $g(n) = \log(n)/\log(2)$. They differ by a constant factor, so $f = \Theta(g)$.
2. $f(n) = (\log n)^{20}, g(n) = n$. We have

$$\lim_{n \rightarrow \infty} \frac{(\log n)^{20}}{n} = \lim_{n \rightarrow \infty} \frac{20 \cdot (\log n)^{19} \cdot \frac{1}{n}}{1} = \dots = \lim_{n \rightarrow \infty} \frac{20!}{n} = 0 \implies f = O(g) \quad (10)$$

3. $f(n) = n^{100}, g(n) = 1.01^n$. We have

$$\lim_{n \rightarrow \infty} \frac{n^{100}}{1.01^n} = \lim_{n \rightarrow \infty} \frac{100n^{99}}{1.01^n \cdot \log(1.01)} = \dots = \lim_{n \rightarrow \infty} \frac{100!}{1.01^n \cdot (\log 1.01)^{100}} = 0 \implies f = O(g) \quad (11)$$

Let's do a slightly more nontrivial example.

Example 1.2 ()

Given the following algorithm, what is the runtime?

```

1  for i in range(1, n+1):
2      j = 1
3      while j <= i:
4          j = 2 * j

```

Now we can see that for each i , we will double up to $\log_2(i)$ times. Therefore summing this all over i is

$$\sum_{i=1}^n \log_2(i) = \log_2(n!) \leq \log_2(n^n) = n \log_2(n) \quad (12)$$

and so we can see that the runtime is $O(n \log n)$. Other ways to do this is to just replace the summation with an integral.^a

$$\int_1^n \log_2(x) dx = x \log(x) - x \Big|_1^n = n \log(n) - n + 1 = O(n \log n) \quad (13)$$

1.1 Recursive Algorithms and Recurrence Relation

I assume that the reader is familiar with recursive algorithms. Now to evaluate the runtime of a recursive algorithm, one must implicitly solve for the runtime of its recursive calls.

^aNeed more justification on why this is the case. Mentioned in lecture.

2 Brute Force Algorithms

2.1 Basic Arithmetic

In here, we use basic deductions from elementary algebra to give us a starting point at which we analyze fundamental arithmetic algorithms.

Theorem 2.1 (Complexity of Addition)

The complexity of addition of two $O(N)$ values with n bits is

1. $O(n)$ bit complexity.
2. $O(\log N)$ complexity.
3. $O(1)$ memory complexity.

By the same logic, the complexity of subtraction is

1. $O(n)$ bit complexity.
2. $O(\log N)$ complexity.
3. $O(1)$ memory complexity.

Proof.

To see bit complexity, we are really taking each bit of each number and adding them together, plus a potential carry operation. Therefore, we are doing a bounded number of computations per bit, which is $O(1)$, but we must at least read through all of the bits, making this $O(\max\{n, m\})$.

Theorem 2.2 (Complexity of Multiplication)

The complexity of multiplication of two values N, M with bits n, m is

1. $O(n^2)$ bit complexity.^a
2. $O((\log n)^2)$ complexity.
- 3.

Theorem 2.3 (Complexity of Division)

The complexity of multiplication of two values N, M with bits n, m is

1. $O(n^2)$ bit complexity.
- 2.

Theorem 2.4 (Complexity of Modulus)

The complexity of multiplication of two values N, M with bits n, m is

1. $O(n^2)$ bit complexity.
- 2.

Theorem 2.5 (Complexity of Exponentiation)

The complexity of multiplication of two values N, M with bits n, m is

1. $O(n^2)$ bit complexity.
- 2.

^aIt turns out we can do better, which we will learn later.

Theorem 2.6 (Complexity of Square Root)

The complexity of multiplication of two values N, M with bits n, m is

1. $O(n^2)$ bit complexity.
- 2.

Definition 2.1 (Factorial)

2.2 Lists

Definition 2.2 (Max and Min of List)**Definition 2.3 (Bubble Sort)****Definition 2.4 (Binary Search)**

2.3 Stack, Queues, Heaps

A heap is sort of in between a sorted array and an unsorted array.

2.4 Cryptography

Example 2.1 (GCD of Two Numbers)

Take a look at the following algorithm.

```
1 def gcd(a, b):
2     if a == b:
3         return a
4     elif a > b:
5         return gcd(a - b, b)
6     else:
7         return gcd(a, b - a)
8
9 print(gcd(63, 210))
```

Definition 2.5 (Primality Testing)**Definition 2.6 (Integer Factorization)**

2.5 Matrix Operations

Definition 2.7 (Matrix Multiplication)

Definition 2.8 (Singular Value Decomposition)

Definition 2.9 (QR Decomposition)

Definition 2.10 (LU Decomposition)

Definition 2.11 (Matrix Inversion)

3 Divide and Conquer

Definition 3.1 (Divide and Conquer Algorithms)

3.1 Karatsuba Algorithm for Multiplication

3.2 Merge Sort

3.3 Strassen Algorithm

3.4 Fast Fourier Transform

4 Hashing and Probabilistic Algorithms

4.1 Modulo Operations

4.2 Hashing

4.3 Primality Testing

5 Dynamic Programming

5.1 Longest Increasing Subsequence

5.2 Knapsack

6 Graphs

A huge portion of problems can be solved by representing as a *graph* data structure. In here, we will explore various problems that can be solved through *graph algorithms*.

6.1 Representations and Properties

All graphs consist of a set of vertices/nodes V and edges E . This tuple is what makes up a graph. We denote $|V| = n, |E| = m$.

Definition 6.1 (Undirected Graphs)

An **undirected graph** $G(V, E)$ is a tuple, where $V = \{v_1, \dots, v_n\}$ is the vertex set and $E = \{\{v_i, v_j\}\}$ is the edge set (note that it is a set of sets!).

1. The **degree** d_v of a vertex v is the number of edges incident to it.
2. A **path** is a sequence of vertices where adjacent vertices are connected by a path in E . It's **length** is the number of edges in the path.
3. A **cycle/circuit** is a path that has the same start and end.
4. A graph is **connected** if for every pair of vertices $e_i, e_j \in E$, there is a path from e_i to e_j .
5. A **connected component** is a maximal subset of connected vertices.

Definition 6.2 (Directed Graph)

A **directed graph** $G(V, E)$ is a tuple, where $V = \{v_1, \dots, v_n\}$ is the vertex set and $E = \{(v_i, v_j)\}$ is the edge set (note that it is a set of tuples, so $(i, j) \neq (j, i)$).

1. The **in/out degree** $d_{v,i}, d_{v,o}$ of a vertex v is the number of edges going in to or out from v .
2. A **path** is a sequence of vertices where adjacent vertices are connected by a path in E . It's **length** is the number of edges in the path.
3. A **cycle/circuit** is a path that has the same start and end.
4. A directed graph is **strongly connected** if for every pair of vertices $e_i, e_j \in E$, there is a path from e_i to e_j .^a
5. A **strongly connected component** is a maximal subset of connected vertices.

In fact, from these definitions alone, we can solve an ancient puzzle called *the Bridges of Königsberg*. Euler, in trying to solve this problem, had invented graph theory.

Example 6.1 (Bridges of Königsberg)

Is there a way to walk that crosses each bridge *exactly* once?

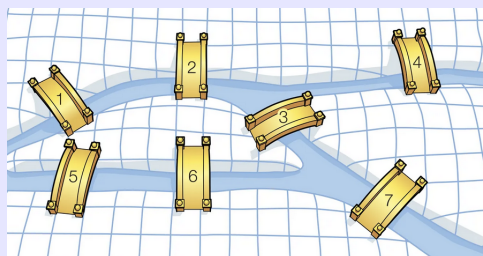


Figure 1: Bridges of Königsberg

It can be decomposed into this undirected graph.

^aObviously, a connected undirected graph is also strongly connected.

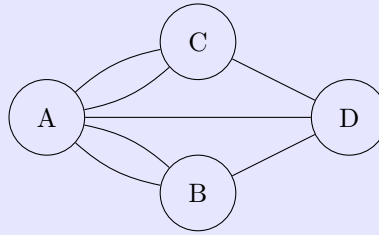


Figure 2: Graph representation.

Euler's observation is that except for start and end points, a walk leaves any vertex by different edge than the incoming edge. Therefore, the degree (number of edges incident on it) must have an even number, so all but 2 vertices must have an even degree. Since every vertex has an odd degree, there is no way of doing it.

In addition to the *adjacency list* representation, another way in which we represent a directed graph is through *adjacency matrices*.

Definition 6.3 (Adjacency Matrix)

In a finite directed graph (V, E) , we can construct a bijection from V to the natural numbers and so we label each element in V with $i \in \mathbb{N}$. Then, we can construct a matrix A such that

$$A_{ij} = \begin{cases} 1 & \text{if } (i, j) \in E \\ 0 & \text{if } (i, j) \notin E \end{cases} \quad (14)$$

While the adjacency matrix does have its advantages and has a cleaner form, usually in sparse graphs this is memory inefficient due to there being an overwhelming number of 0s.

Definition 6.4 (Trees)

An undirected graph $G(V, E)$ is a **tree** if

1. G is connected.
2. G has no cycles.^a

Removing the first requirement gives us the definition of a **forest**, which is a collection of trees. Conversely, if $G(V, E)$ is connected and $|E| = n - 1$, then G is a tree.

Theorem 6.1 (Properties of Trees)

If $G(V, E)$ is a tree, then

1. There exists a $v \in V$ s.t. $d_v = 1$, called a **leaf node**.
2. $|E| = |V| - 1 = n - 1$.

Proof.

The outlines are quite intuitive.

1. There must be some leaf node since if there wasn't, then we would have a cycle. We can use proof by contradiction.
2. We can use proof by induction. We start off with one vertex and to construct a tree, we must add one edge and one vertex at every step, keeping this invariant.

^aThis makes sense, since to get back to a previous vertex you must backtrack.

6.2 Exploration

Given two $v, s \in V$ either directed or undirected, how can we find the shortest path from v to s ? We can do with either with DFS or BFS.

Definition 6.5 (DFS)

The recursive algorithm is

```
1 visited = set()
2 def dfs(start):
3     if start not in visited:
4         visited.add(start)
5         # do something
6         neighbors = ...
7         for neighbor in neighbors:
8             dfs(neighbor)
```

The iterative algorithm uses a stack, which mirrors the function call stack.

```
1 visited = set()
2
3 def dfs(start):
4     toExplore = []
5     current = start;
6     toExplore.append(current)
7     visited.add(current)
8     while toExplore:
9         current = toExplore.pop()
10        # Do something
11        neighbors = ...
12        for neighbor in neighbors:
13            if neighbor not in visited:
14                visited.add(neighbor)
15                toExplore.append(neighbor)
```

Theorem 6.2 (Runtime of DFS)

The runtime of DFS is $O(n + m)$.

Proof.

Definition 6.6 (BFS)

The iterative version is shown.^a

```
1 visited = set()
2 def bfs(start):
3     toExplore = collections.deque()
4     current = start;
5     toExplore.append(current)
6     visited.add(current)
7     while toExplore:
8         current = toExplore.popleft()
```

```
9      # Do something
10     neighbors = ...
11     for neighbor in neighbors:
12         if neighbor not in visited:
13             visited.add(neighbor)
14             toExplore.append(neighbor)
```

Theorem 6.3 (Runtime of BFS)

The runtime of BFS is $O(n + m)$.

Proof.

To get the running time, we know that each vertex is popped only once from the queue, giving us $O(n)$. For each pop, we are exploring all the neighbors of V .

$$O\left(\sum_{v \in V} |\text{neighbors of } v| + 1\right) = O\left(\sum_{v \in V} d_v + 1\right) \quad (15)$$

$$= O(2|E| + |V|) = O(m + n) \quad (16)$$

which is linear in input size!

The more straightforward application is in reachability.

Example 6.2 (Reachability)

Given a directed graph and a node v , find all nodes that are reachable from v .

Exercise 6.1 ()

Prove that in any connected undirected graph $G = (V, E)$ there is a vertex $v \in V$ s.t. G remains connected after removing v .

Proof.

You can make a BFS tree from this graph, and there has to be a last layer. Just remove the node from this layer.

Exercise 6.2 ()

Give an example of a strongly connected directed graph $G = (V, E)$ s.t. that every $v \in V$, removing v from G gives a directed graph that is not strongly connected.

Exercise 6.3 (DPV 3.16)

^aThe recursive version of BFS is very nontrivial.

Proof.

Do BFS but now recursively store the maximum of all the prerequisite courses plus 1 for the current course.

6.3 Directed Acyclic Graphs and Topological Sorting

Definition 6.7 (Directed Acyclic Graph)

A DAG is a directed graph that has no cycles. Note that a DAG must have a node that has no in-edges.

To determine if a graph is a DAG, then we can brute force it by taking a node $s \in V$, running DFS/BFS, and if a neighbor is already in visited, return False. Then go through this for all starting nodes $s \in V$. This again has quadratic runtime. Can we do better? This introduces us to topological sorting.

It may be helpful to take a graph $G(V, E)$ and induce some partial order on the set of nodes V based off of E . It turns out that we can do this for a specific type of graph.

Definition 6.8 (Topological Sort)

Given a directed acyclic graph (DAG), a linear ordering of vertices such that for every directed edge $u \rightarrow v$, vertex u comes before v in the ordering is called a **topological sort**. It satisfies the facts:

1. The first vertex must have an in-degree of 0.
2. A topological sort is not unique.

Example 6.3 (Simple Topological Sort)

The graph below

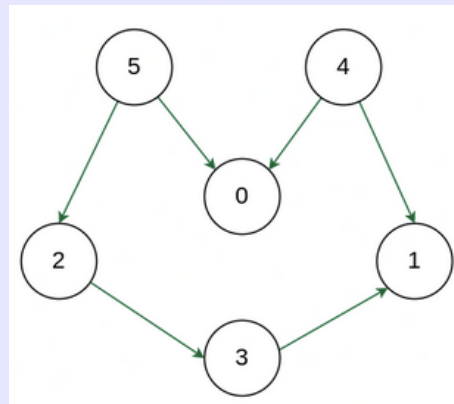


Figure 3

can have the two (not exhaustive) topological sortings.

1. [5, 4, 2, 3, 1, 0]
2. [4, 5, 2, 3, 1, 0]

To determine if a graph is a DAG, note the following theorem.

Theorem 6.4 (Topological Order and DAGs)

G has a topological order if and only if it is a DAG.

Proof.

To prove that a DAG has a topological order, we use induction. Pick a v such that its indegree is 0. Then, delete v , and therefore $G \setminus v$ is also a DAG with a topological order since we are only deleting edges. We keep going.

Therefore, if we can successfully topologically sort, we know it is a DAG. So we can kill two birds with one stone. Let's see how this is implemented. We can do it iteratively and recursively (the proof above should hint that this can be recursive).

Algorithm 6.1 (Iterative Topological Sort, Determine If Graph is DAG)

The general idea is that we first find the node that has 0 in-degree. From here, we can do DFS, and when we run out of neighbors to explore, then we push this into a queue. This is essentially a post-order traversal, where at the end are going to be the end nodes with no more neighbors, and the node we started from will be added last. Then we loop through and do this for all start nodes. We first need a slightly modified form of DFS.

Require: Nodes V , adjacency list E

```

1: visited ← set()
2: res ← stack()
3: is_acyclic ← True
4: function DFS( $v \in V$ )
5:   if  $v \neq$  visited then
6:     add  $v$  to visited
7:      $N_v \leftarrow$  neighbors of  $v$ 
8:     for  $n \in N_v$  do
9:       if  $n \in$  visited then
10:        is_acyclic ← False
11:      end if
12:      DFS( $n$ )
13:    end for
14:    push  $v$  onto res
15:  end if
16: end function
17:
18: function TOPOLOGICALSORT( $V, E$ )
19:   for  $v \in V$  do
20:     DFS( $v$ )
21:   end for
22:   if ! is_acyclic then
23:     return False
24:   end if
25:   return reversed of res
26: end function

```

Note that this runtime is $O(|V| + |E|)$ since we are just running DFS with a constant amount of work on top of each call.

Algorithm 6.2 (Recursive Topological Sort)

We want to see that while G is nonempty, we want to find the $v \in V$ such that it has indegree 0. Then place v next in order, and then delete v and all edges out of v . The problem is finding which vertex has indegree 0 (if we brute force it by looking through all remaining nodes and edges, you have quadratic runtime). To do this fast, the idea is

1. initially scan over all edges to store the indegrees of every node to a list `indeg`.
2. store all nodes with indegree 0 to a queue.
3. Run through the queue, and during each loop, when we remove a node, we look at all of its out-nodes s and decrement `indeg[s]`. If `indeg[s] = 0`, then add it to the queue.

Require: Nodes V , Edges E

```

1:  $q \leftarrow \text{queue}()$ 
2:  $\text{indeg} \leftarrow \text{list}()$ 
3:  $\text{visited} \leftarrow 0$ 
4: function RECUR( $x$ )
5:   initialize the  $\text{indeg}$  and  $q$ 
6:   while  $q$  is nonempty do
7:      $v \leftarrow \text{pop}(q)$ 
8:      $\text{visited} += 1$ 
9:     for each  $w \in E[v]$  do
10:       $\text{indeg}[w] -= 1$ 
11:      if  $\text{indeg}[w] = 0$  then
12:        push  $w$  into  $q$ 
13:      end if
14:    end for
15:  end while
16:  if  $\text{visited} \neq |V|$  then
17:    return False
18:  end if
19:  return True
20: end function

```

Notice that the inner for loop is $O(d(v) + 1)$, while we run over all n . So really, we are doing $O(n(d(v) + 1)) = O(m + n)$, where the plus n comes from the constant work we are doing for each node. Note that if we have a non-DAG, then at some point the queue will be empty but we haven't processed all the vertices, at which point we can declare failure.

To end this, we can make a general statement about all directed graphs.

Theorem 6.5 ()

Every directed graph is a DAG of strongly connected components (SCC).

This gives us a way to represent a directed graph with a collection of DAGs.² An extension of topological sort is making a *BFS tree*, which partitions a graph into layers that represent the number of steps required to go from a source vertex to a node.

²In fact, this Kosaraju's algorithm, can be done in linear time, though it is highly nontrivial.

Algorithm 6.3 (BFS Tree)

To construct a BFS tree, we just need to slightly modify the original BFS code.

Require: Nodes V , adjacency list E

```

1: visited = set()
2: layers = {v : 0 | v ∈ V}
3: function BFS(start)
4:   layer ← 0
5:   toExplore ← queue()
6:   add (start, layer) to toExplore
7:   add start to visited
8:   while toExplore do
9:     curr, layer = pop from toExplore
10:    layers[curr] = layer
11:    for n ∈ neighbors of curr do
12:      if n ∉ visited then
13:        add n to visited
14:        add (n, layer + 1) to toExplore
15:      end if
16:    end for
17:  end while
18: end function

```

This is simply BFS with constant extra work so it is $O(n + m)$.

So, a BFS tree is really just another way to topologically sort. Note the following properties.

1. In a directed graph, no nodes can jump from layer i to layers $j > i + 1$, since if it could, then it would be in layer $i + 1$. However, nodes can jump from layer j back to any layer $i < j$, even skipping layers.
2. In a directed graph, going forward is the same as going back, so nodes can jump at most one layer forwards or backwards.

6.4 Bipartite Graphs

Now we shall see a further application of BFS trees.

Definition 6.9 (Bipartite Graph)

A **bipartite graph** is an undirected graph $G(V, E)$ where we can partition $V = L \sqcup R$ such that for all $e = \{u, v\} \in E$, we have $u \in L, v \in R$.

We would like to devise some method to determine if an arbitrary graph is bipartite.

Theorem 6.6 ()

G is bipartite if and only if all cycles in G are even length.

Proof.

Proving (\implies) is quite easy since if we suppose G has an odd length cycle, then we start packing vertices of a cycle into L, R , but by the time we came back to the start, we are forced to pack it into

the wrong partition!

The converse is quite hard to prove, and we'll take it at face value.

Now in practice, how would we determine if all cycles are even length? This is where BFS shines.

Algorithm 6.4 (Determine Bipartite On All Cycles of Even Length)

The general idea is we first run BFS on the graph starting at $s \in V$, which divides it up into layers L_1, \dots, L_l representing the shortest path from s . Then for each layer $L_i \subset V$, we check if there are connections between two vertices $x, y \in L_i$. If there are connections, then this is not bipartite. If there are none, then this is bipartite since we can then color it.

```

Require: Nodes  $V$ , adjacency list  $E$ 
1: visited = set()
2: layers = { $v : 0 \mid v \in V$ }
3: function BFS(start)
4:   layer  $\leftarrow 0$ 
5:   toExplore  $\leftarrow$  queue()
6:   add (start, layer) to toExplore
7:   add start to visited
8:   while toExplore do
9:     curr, layer = pop from toExplore
10:    layers[curr] = layer
11:    for  $n \in$  neighbors of curr do
12:      if  $n \notin$  visited then
13:        add  $n$  to visited
14:        add ( $n, layer + 1$ ) to visited
15:      end if
16:    end for
17:  end while
18: end function
19:
20: function BIPARTITE( $V, E$ )
21:   BFS( $v$ ) for some  $v \in V$ 
22:   for  $(u, v) \in E$  do
23:     if layers[ $u$ ] == layers[ $v$ ] then
24:       return False
25:     end if
26:   end for
27:   return True
28: end function

```

Therefore, we run BFS, which is $O(n + m)$, and then to compare the edges, it is $O(m)$.

Bipartiteness is actually a special case of *coloring problems*. Given a graph with k colors, can I color it so that every neighbor has a different color than the original node? It may seem like at first glance that we can do the same method and look at the layers again, but it turns out that 3-coloring is hard. More specifically it is an NP-complete problem, which colloquially means that there isn't much of a better way than a brute-force solution. However, it turns out that according to the *4 color theorem*, any map can be colored with 4 colors.

6.5 Strongly Connected Graphs

Now how do we find out if a directed graph is strongly connected? The straightforward solution would be to take each vertex $v \in V$, run BFS to find the set of vertices reachable from v , and do this for every vertex. The total running time is $O(n(n+m))$, which is quadratic. Note that for an undirected graph this is trivial since we just run DFS/BFS once.

Theorem 6.7 ()

G is strongly connected if and only if for any $v \in V$,

1. all of V is reachable from v .
2. v is reachable from any $s \in V$

Algorithm 6.5 (Determine if Graph is Strongly Connected)

Using the theorem above, we can run BFS/DFS twice: one on the original graph and one on the reversed graph, consisting of all edges directed in the opposite direction.

Require: Nodes V , Adjacency list E

```

1: function STRONGLYCONNECTED( $s \in V$ )
2:   visited  $\leftarrow$  set()
3:   BFS( $s$ )
4:   if visited  $\neq V$  then
5:     return False
6:   end if
7:   visited  $\leftarrow$  set()
8:   reverse all edges in  $E$ 
9:   BFS( $s$ )
10:  if visited  $\neq V$  then
11:    return False
12:  end if
13:  return True
14: end function

```

The running time is just running BFS twice plus the time to reverse the edges, so it is $O(n+m)$.

6.6 Shortest Path

In the shortest path, you are given a *weighted* (positive integer) directed graph and your goal is to find a path from s to t with the smallest length. This is where we use Dijkstra's. What we can do to brute force is just replace a edge with length k to k edges of length 1, and we run BFS on this. However, this is not efficient. This is where we introduce Dijkstra. The following is how it is introduced in class.

Algorithm 6.6 (Primitive Dijkstra)

We can keep a temporarily list π of the shortest path we have found so far, and a permanent list **dist** keeping track of all paths we know are for sure the shortest path.

Require: Graph $G(E, V)$

```

1:  $S \leftarrow \{s\}$                                 ▷set of nodes that we know for sure is shortest
2:  $\text{dist}[s] = 0$  and the rest very large numbers    ▷our final list
3:  $\pi[v] = w_{sv}$  for all  $v \in V$                     ▷initialize list with neighboring nodes from start  $s$ 
4: function DIJKSTRA( $s$ )
5:    $u = \text{argmin}_{v \notin S} \pi[v]$                 ▷Find node having minimum accum weight so far
6:   add  $u$  to  $S$                                 ▷This node must be shortest so add to  $S$ 
7:    $\text{dist}[u] = \pi[u]$                             ▷Now we can update its shortest path in dist
8:   for  $v \notin S$  do                            ▷Look at all neighbors of  $u$  and update those not in
9:      $\pi[v] \leftarrow \min\{\pi[v], d[u] + w_{uv}\}$     ▷ $S$  since those in  $S$  are all guaranteed to be shortest
10:  end for
11: end function

```

The problem is line 5 above. We don't want this linear search time since it makes the whole thing quadratic, so rather than a list, we can implement a heap, resulting in the code below.

Algorithm 6.7 (Dijkstra's Algorithm)

The general idea is to run a graph traversal like BFS but when you reach a new vertex v , you can store the accumulated time it took to get to v and store for all neighbors the accumulated time it will take to get to each of those neighbors. If it is less than what we have currently, then we have found a shorter path and we should update this.

Require: Nodes V , Edges E

```

1: function DIJKSTRA( $s$ )
2:    $\text{dist} \leftarrow$  list of size  $|V|$  with  $+\infty$     ▷Initialize a list of large numbers
3:    $\text{dist}[s] \leftarrow 0$                             ▷The starting node has dist 0
4:    $\text{predecessors} \leftarrow \{v : \text{None} \mid v \in V\}$ 
5:    $\text{toExplore} \leftarrow \text{minheap}()$                 ▷A priority queue of (weight, node)
6:   add  $(0, s)$  to  $\text{toExplore}$ 
7:   while  $\text{toExplore}$  do
8:      $(\text{curr\_dist}, \text{curr\_node}) \leftarrow$  pop from  $\text{toExplore}$ 
9:     if  $\text{curr\_dist} > \text{dist}[\text{curr\_node}]$  then
10:      continue
11:    end if
12:    for  $\text{neighbor}, \text{weight} \in E[\text{curr}]$  do
13:       $\text{new\_dist} \leftarrow \text{curr\_dist} + \text{weight}$ 
14:      if  $\text{new\_dist} < \text{dist}[\text{neighbor}]$  then
15:         $\text{dist}[\text{neighbor}] = \text{new\_dist}$ 
16:         $\text{predecessors}[\text{neighbor}] = \text{curr\_node}$ 
17:        push  $(\text{new\_dist}, \text{neighbor})$  onto  $\text{toExplore}$ 
18:      end if
19:    end for
20:  end while
21:  return distances, predecessors
22: end function

```

You essentially push n times and pop m times, and the time per push and pop is $\log_2(n)$. Therefore, the total time to push is $n \log(n)$ and to pop is $m \log(n)$, making the total runtime $O(\log(n)(n + m))$.

The first example gotten in class ignores the distances and just attempts to modify the distances in the heap itself (through the decrease key operation). This takes $2 \log_2(n)$, but if we use a heap with d children, we

can modify the runtime to $d \log_d(n)$. Therefore, the total runtime with tunable parameter d is

$$O((m + nd) \log_d(n)) \quad (17)$$

which can be minimized if we set $d = m/n$, so $O(m \log_{m/n} n)$, where for dense graphs m/n is large and so it can behave roughly in linear time $\Theta(m)$.

6.7 Negative Weighted Graphs

Now let's extend this problem to find the shortest path in negative weighted graphs. Before we think of a solution, we must make sure that there is no cycle that has a negative accumulated path. Otherwise, this problem becomes ill-defined, so we first assume that such a shortest path exists.

At first glance, we may just think of adding $\min(v)$, the minimum value to every node so that this now just becomes a regular positive graph and run BFS on it. However, this does not work since we are not adding a constant number over all paths (it is proportional to the number of nodes in the path).

Another way we can think of is just run Dijkstra. However, if it is looking at two paths. We can have $s \xrightarrow{2} b$ and $s \xrightarrow{5} a \xrightarrow{-4} b$. Dijkstra will immediately go to b thinking that it is the shortest path, since that's how far it see. So we need to look far into the future. Therefore, after an arbitrarily long path length, you could get a negative length that just kills your accumulator.

Another way we can do is to use dynamic programming.

Theorem 6.8 (Bellman Equations)

We write the **Bellman equations**.

$$d[v] = \min_w \{d[w] + l_{wv}\} \quad (18)$$

with $d[s] = 0$ for the starting vertex. The solution has a unique solution that finds the shortest path from s to any $v \in V$.

Proof.

Note that $d[w] + l_{wv}$ is the length from some path from $s \mapsto v$ that goes through w . The minimum of it must be the shortest path over all $w \in V$. Suppose the shortest path goes through fixed x . If there exists a shorter path from $s \mapsto x$, then replace $d[x]$ by this shortest path. Therefore,

$$d[v] = d[x] + l_{xv} \leq d[w] + l_{wv} \implies d[v] = \min_w \{d[w] + l_{wv}\} \quad (19)$$

To prove uniqueness, suppose there are some other solutions π where $\pi[v] \neq d[v]$ for some v . But this cannot be the case by definition since $d[v] \leq \pi[v]$ for all v .

Theorem 6.9 ()

Given the shortest paths, we can lay out this graph like a tree where $l_{ab} = l_{aa_1} + l_{a_1a_2} + \dots + l_{a_ib}$.

So how do we actually implement this?

Algorithm 6.8 (Shortest Path in Possibly Negative Weighted Graph)

Require: Nodes V , Edges E

```

1: function SHORTPATH( $V, E$ )
2:    $\text{res} \leftarrow \text{list}(0)$  of large numbers of size  $|V|$ .
3:    $\text{res}[s] = 0$ 
4:    $\text{predecessors} \leftarrow \{v : \text{None} \mid v \in V\}$ 
5:   while  $\exists(u, v)$  s.t.  $\text{res}[v] > \text{res}[u] + l_{uv}$  do
6:      $\text{res}[v] \leftarrow \text{res}[u] + l_{uv}$ 
7:      $\text{predecessor}[v] \leftarrow u$ 
8:   end while
9: end function

```

This is guaranteed to converge and stop after a finite number of steps since at every iteration, a path will either

1. get updated from infinity to a path length
2. get reduced from a path length to a shorter path length

And we will have to reach the shortest path length at which point we can't reduce it further.^a

Computing the runtime is a bit tricky, since we can look at the same edge twice since minimum paths may have been updated in the middle. Therefore this list **res** may reduce very slowly. For example, let the length of each edge $|l_e| \leq L$. Then in the worst case, $\text{res}[s]$ can be initialized to $(n-1)L$ representing the max path across all nodes, and we can decrease by 1 in each step. So over all nodes, we can decrease so that each $\text{res}[s]$ becomes $-(n-1)L$, meaning that we are doing on the order of $2n^2L$ iterations. This is too slow, especially for non-distributed settings.

A better way is to not be so random about how we choose the (u, v) in the while loop. Notice how we can lay out the shortest paths like a tree, so we can work in layers. The next algorithm implements this.

Algorithm 6.9 (Bellman-Ford Algorithm)

We think of going in rounds indexed by t , and at every round, we are iterating through all the nodes and updating the shortest path of v using the shortest path of w included in all in-neighbors of v . At most, we will need to update this at most n times, which will guarantee convergence.

Require: Nodes V , Edges E

```

1:  $\pi \leftarrow \text{list}(0)$  of large numbers of size  $|V|$ .
2:  $\pi[s] = 0$ 
3: function BELLMANFORD( $x$ )
4:   for  $t = 1, \dots, n-1$  do
5:     for  $v \in V$  do
6:        $\pi^{(t)}[v] \leftarrow \min_w \{\pi^{(k-1)}[v], \pi^{(k-1)}[w] + l_{wv}\}$ 
7:     end for
8:   end for
9: end function

```

The runtime is easier to see.

1. The step in the inner loop looks over the set of nodes of size $\text{indeg}(v)$.
2. Looping over all the nodes in the inner for loop means that we are going over all edges, so $O(m)$.
3. The outer for loop goes through $n-1$ times, so the total runtime is $O(nm)$.

^aThis algorithm is also called *policy iteration* in reinforcement learning and is analogous to gradient descent.

At first glance, this problem seems like it isn't too different from Dijkstra, but there is a 50-year conjecture that this cannot be improved to linear time.

6.8 Minimum Spanning Trees

Definition 6.10 (Spanning Tree)

Given an undirected graph $G(V, E)$, a **spanning tree** is a subgraph $T(V, E' \subset E)$ that is

1. a tree, and
2. spans the graph, i.e. is connected

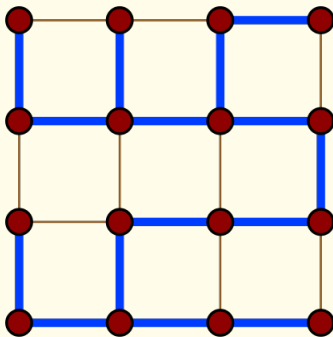


Figure 4: A spanning tree on a 4×4 grid graph.

Note that an unconnected graph will never have a spanning tree, but what about a connected graph?

Theorem 6.10 (Spanning Trees of Connected Graphs)

A connected graph will always have at least one spanning tree, not necessarily unique.

Given a connected undirected weighted graph, we may want to find the **minimum spanning tree (MST)**, i.e. the spanning tree with edges E' such that the sum of the weights of all $e \in E'$ is minimized.³ How do we do this? There are two well-known algorithms to solve this. Prim's and Kruskal's algorithm.

6.8.1 Prim's Algorithm with Cuts

Let's try to apply what we already know: Dijkstra. If we run Dijkstra on the graph starting at $s \in V$, we can get the shortest path from s to every other node in the graph. This will give us a tree, but it may not be minimum.

³An application of this is when we generally want to make sparse graphs. In a datacenter, wires can be expensive, so how I can minimize the length of wires to buy to construct a spanning subgraph?

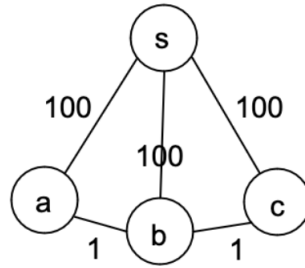


Figure 5: If we run Dijkstra on s , then our output will be a tree of cost 300, even when the actual MST can be of cost 102 starting from a .

It may seem like this is just a problem of where we start, but even this is not the case.

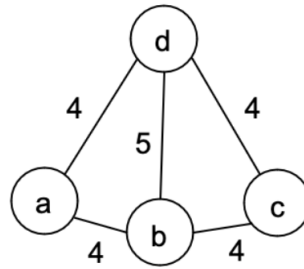


Figure 6: No matter where we start from, we will never output the MST. The MST has cost 12. If we start from b or d , we will get a tree of cost 13. If we start from a or c , we will get a tree of cost 16.

Definition 6.11 (Cuts)

Given graph $G(V, E)$, a **cut** is a partitioning of V into $(S, V \setminus S)$. Furthermore, let $\text{Cut}(S)$ be the number of edges with exactly one endpoint in S and the other in $V \setminus S$.

Theorem 6.11 (Cycles and Cuts)

Given cycle $C \subset E$ in a graph and a cut $S \subset V$,

$$|C \cap \text{Cut}(S)| \quad (20)$$

is even. We can intuit this by visualizing the cycle as a long piece of looped string and a cut is a circle. The intersection between this circle and the string must be even since every time the cycle crosses through the cut, it must return back across the cut to the initial point.

Now time for a bizarre theorem.

Theorem 6.12 (Cut Property of MSTs)

For all cuts $S \subset V$ of an undirected graph, the minimum cost edge in $\text{Cut}(S)$ belongs to the MST. Furthermore, the converse is true: if we take all cuts and find all their minimum cost edges, these edges is precisely the MST! Therefore, an edge $e \in \text{MST}$ iff e is a min-cost edge for some cut.

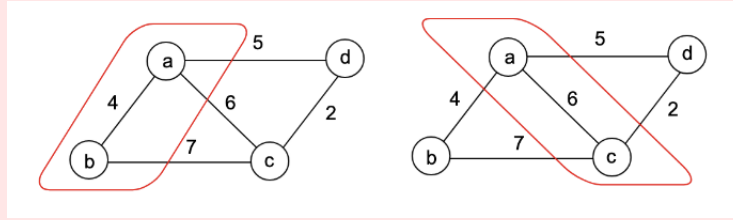


Figure 7: In the left cut, the edges are (a, d) , (b, c) , (a, c) . The minimum weight is 5 on the (a, d) edge, so it must be in the MST. For the right cut, (c, d) must be in the MST.

The final part is that if we have all edge costs different, then we will have a *unique* MST.

Proof.

We use a greedy approach and prove by contradiction. Suppose that this is not true, i.e. there exists a cut S with minimum cost edge e , and $e \notin \text{MST}$. Then, there exists some other edge $e' \in \text{Cut}(S)$ that is in the MST, since the MST is spanning and it must cross over to connect the whole graph. Well if we just put e in and take e' out, we will still have a spanning tree since it connects the left spanning tree to the right spanning tree, and we now have a cheaper tree. So the original cannot be the MST in the first place.

To prove the converse, consider some edge e in the MST and we must prove that it is the minimum cost edge in some cut. Note that if we take e out, then it divides the MST into two connected components, and we can just define the cut as these subsets of nodes. So this is in $\text{Cut}(S)$ for some $S \subset V$. We can also prove that this is minimal since if it wasn't the minimum cost edge for some cut, we could have taken it out and inserted a cheaper edge e' to begin with, getting a cheaper spanning tree.

Algorithm 6.10 (Primitive Prim's Algorithm)

We can just brute force this logic into an algorithm, which is not efficient.

Require: Graph $G(V, E)$

$r \leftarrow \{\}$

function SOLVE(x)

for all $S \subset V$ **do**

 add min-cost edge in $\text{Cut}(S)$ to r

end for

return r

end function

It is clear that a cut is defined by a subset of S , so really the number of cuts a graph can have is $2^{|S|}-1$, which is exponential in n . However, the minimum spanning tree isn't exponential since it must have $n - 1$ edges, so there must be many cuts with the same minimum edge.

One way is to start with one vertex a that contains the minimum cost edge (a, b) across all edges. This edge must be minimal and must be in the MST. Then we can look at the cut $S = \{a, b\}$ and look at that cut. We keep doing this, keeping track of the set of edges we need to look at after adding a new node to our cut. So the number of cuts I consider is equal to the number of edges in the spanning tree.

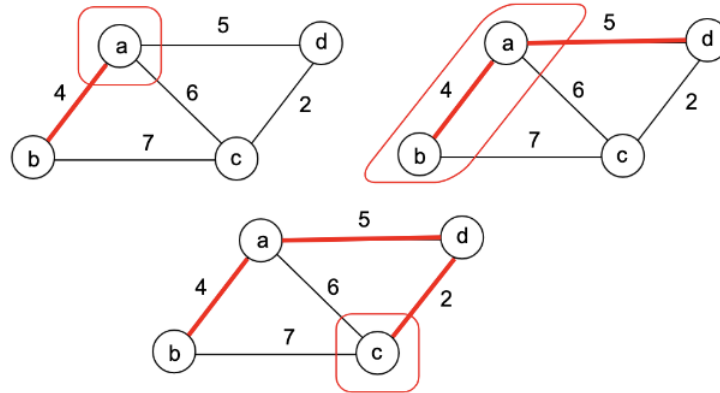


Figure 8: Step by step process of the method we mention above.

Algorithm 6.11 (Prim's Algorithm to Find MST)

It turns out that we can modify Dijkstra to solve it.

Require: Graph $G(E, V)$

<pre> 1: function PRIM(s) 2: $S \leftarrow \{s\}$ 3: $\pi[v] \leftarrow$ list of size V of $+\infty$ 4: $\pi[v] = w_{sv}$ for all $v \in V$ 5: while $S \neq V$ do 6: $u = \operatorname{argmin}_{v \notin S} \pi[v]$ 7: $S \leftarrow S \cup \{u\}$ 8: for $u \notin S$ do 9: $\pi[u] \leftarrow \min\{\pi[u], w_{wu}\}$ 10: end for 11: end while 12: end function </pre>	<p>\trianglerightOur initial cut</p> <p>$\triangleright \pi[u]$ is min cost of getting from u into the S</p> <p>\trianglerightinitialize list with neighboring nodes from start s</p> <p>\trianglerightFind node having minimum cost to reach from S</p> <p>\trianglerightAdding this node to S to expand our cut</p> <p>\trianglerightSince we expanded S, our min reach distances</p> <p>\trianglerightmust be updated. It can only get shorter</p> <p>\trianglerightthrough a path from new u, so compare them</p>
--	--

However, this is not efficient, so we can introduce a minheap to get the argmin step faster.

Algorithm 1 Not completely finished, need to update**Require:** Graph $G(E, V)$

```

1: function PRIM( $s$ )
2:    $S \leftarrow \{s\}$  ▷Our initial cut
3:    $T \leftarrow \text{heap}(\{(u, v, w) \in E \mid u = s\})$  ▷Our heap of edges connected to  $S$ 
4:    $\pi[v] \leftarrow$  list of size  $|V|$  of  $+\infty$  ▷ $\pi[u]$  is min cost of getting from  $u$  into the  $S$ 
5:    $\pi[v] = w_{sv}$  for all  $v \in V$  ▷initialize list with neighboring nodes from start  $s$ 
6:   while  $S \neq V$  do
7:      $u = \text{argmin}_{v \notin S} \pi[v]$  ▷Find node having minimum cost to reach from  $S$ 
8:      $S \leftarrow S \cup \{u\}$  ▷Adding this node to  $S$  to expand our cut
9:     update  $T$ 
10:    for  $v \in \text{neighbors of } u$  do ▷Since we expanded  $S$ , our min reach distances
11:       $\pi[v] \leftarrow \min\{\pi[v], w_{uv}\}$  ▷must be updated. It can only get shorter
12:    end for ▷through a path from new  $u$ , so compare them
13:  end while
14: end function

```

Note that we run through all the nodes in line 6, and in line 10, we run through the neighbors of each edge, making this $O(n + m)$. However, to compute the argmin in line 7, it is a $O(\log n)$ operation, so the total runtime is $O(m + n \log n)$ operation. In class, it says running time is $\Theta(m \log_{m/n} n)$.

6.8.2 Kruskal's Algorithm

If we were to try and construct this algorithm from scratch, we may take a greedy approach by incrementally adding the minimum cost edge from your cut. However, there is one thing to check: have we entered a cycle? Checking whether the next added node a completes a cycle in $S \cup \{a\}$ is nontrivial.

Theorem 6.13 (Cycle Property)

For all cycles C , the max cost edge of C does not belong to MST.

Therefore, you can take S and either add to it using the cut property or delete candidates from it using the cycle property. What is the best order to do this in?

Algorithm 6.12 (Primitive Kruskal's Algorithm)

This algorithm is faster and can be run faster than $O(m \log n)$ time. The general idea is that we sort $e \in E$ in increasing cost, and for each $e \in E$, we use either the cut or cycle property to decide whether e goes in or out.

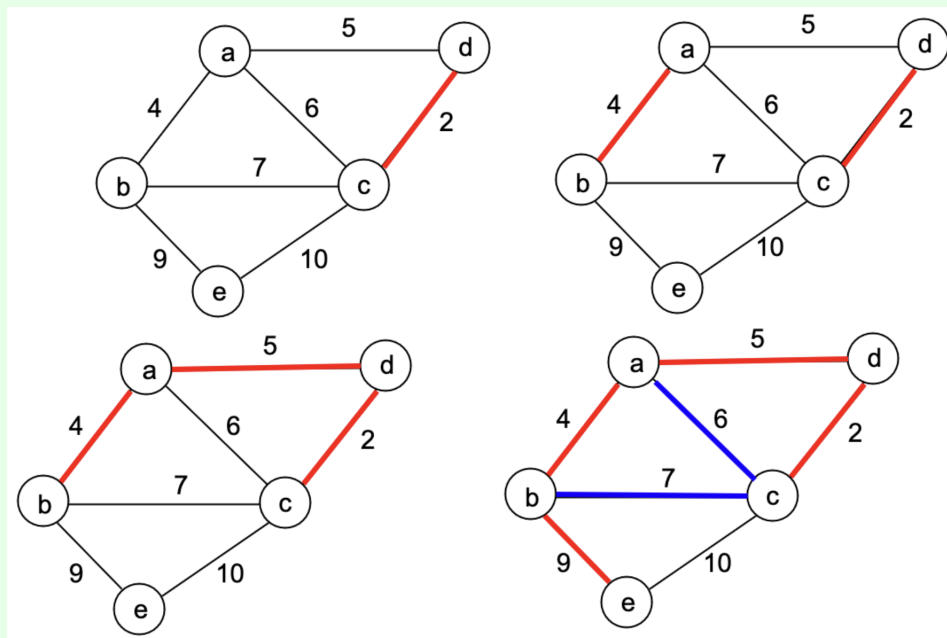


Figure 9: Kruskal's algorithm. In the last step, we see that the next minimum cost edge of 6 and 7 forms a cycle, so we add the edge of length 9.

Require: Graph $G(V, E)$

```

1: function KRUSKAL( $V, E$ )
2:   sort  $E$  in increasing cost
3:    $T \leftarrow \{\}$ 
4:   for  $e \in E$  do
5:     if  $T \cup \{e\}$  does not have cycle then
6:        $T \leftarrow T \cup \{e\}$ 
7:     else
8:       continue
9:     end if
10:  end for
11: end function

```

▷Cut property
 ▷Cycle property
 ▷discard e since from sorting, this edge is heaviest in cycle

The way to prove that this is correct is to show that every step you do is correct, known as *structural induction*, either because of one of the two properties. Say that so far, we have some edges in V which forms a partition of $V = \sqcup_i T_i$ of disjoint trees (can be trees, one edge, or just single nodes). We are looking at the next biggest edge $e = (a, b)$. There are two possibilities.

1. If a, b are both in a single T_i , then this forms a cycle and can be thrown away since this is the max cost edge in the cycle by the cycle property.
2. If a, b connect T_i and T_j for $i \neq j$, then this edge is in $\text{Cut}(T_i)$ and is the minimum cost edge since the rest of the edges in $\text{Cut}(T_i)$ come next in the sorted E . Therefore this must be included by the cut property.

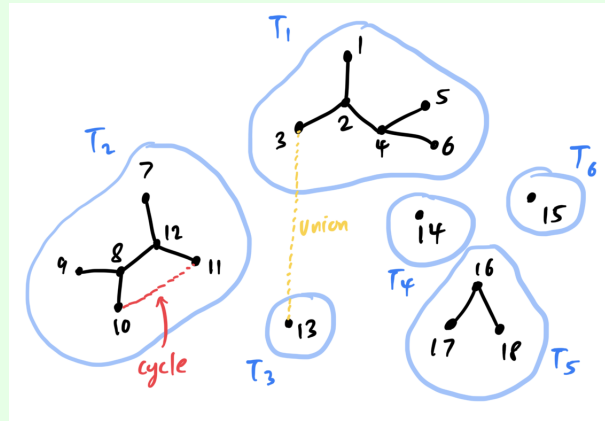


Figure 10: Each T_i is a component formed by the edges chosen so far. For example, $T_1 = \{1, 2, 3, 4, 5, 6\}, \dots$. We can either discard an edge (red) or include an edge (yellow).

The only bottleneck in here is line 5, where we check if e does not complete a cycle in T . It will obviously not be efficient to do BFS, construct a tree, and see if there is a loop by checking if two points in the same layer are connected. It may help to decompose this algorithm into two steps: what is being stored and what is being checked?

Explain the general idea. Note that from our visual, we are really just keeping a set of these points that each make a subtree and connecting them together. How do we efficiently search for which cluster a point is a part of and efficiently merge two clusters? We could use a hashmap but this wouldn't work. We need something like a doubly linked list.

Algorithm 6.13 (Kruskal's Algorithm)

Algorithm 2

Require:

```
function FUNC(x)
end function
```

To analyze the runtime of this, we define the function.

Definition 6.12 (Ackerman Function)

The **Ackerman function** is one of the fastest growing functions known. It is practically infinity.

$$A(m, n) = \begin{cases} n + 1 & \text{if } m = 0 \\ A(m - 1, 1) & \text{if } m > 0 \text{ and } n = 0 \\ A(m - 1, A(m, n - 1)) & \text{if } m > 0 \text{ and } n > 0 \end{cases} \quad (21)$$

The inverse Ackerman function therefore grows extremely slowly.

If we optimize the steps in Kruskal's algorithm, we can get its runtime to

$$O((m + n) \log^*(n)) \quad (22)$$

which is practically linear.

6.8.3 Applications

Here is a way to cluster data, a surprising way to apply MSTs. It is the most widely used application, especially in data science. The problem is that given n data points $x_i \in \mathbb{R}^d$ and an integer k , we want to partition the points into k groups $\mathbf{C} = (C_1, \dots, C_k)$ where $\mathbf{x} = \sqcup_i C_i$. You want to distances between the points within a group to be small and the distances between groups to be large. We can think of finding the objective which takes every pair of clusters and computes the minimum distance between these clusters, and we want to maximize this distance over all pairs of clusters.

$$\operatorname{argmax}_{\mathbf{C}} \min_{p \in C_i, q \in C_j} \{d(p, q)\} \quad (23)$$

Algorithm 6.14 (Single Linkage/Hierarchical Clustering)

The general idea is to take this dense graph, find the MST, and cut off the largest edges from this MST, which will give you k components. This is the answer. Or really, you can use Kruskal's algorithm and terminate earlier when T has k sets/components. Note that as we add edges as we construct our MST, we are merging two clusters into one. So that all you are doing is finding the next pair of closest points and merging the clusters that they are a part of.

Require:

- 1:
- 2: **function** FUNC(\mathbf{x})
- 3: **end function**

Theorem 6.14 ()

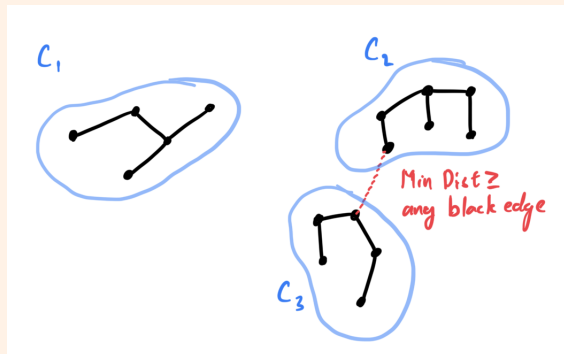
The algorithm above minimizes the objective function.

Proof.

Let \mathbf{C}^* be the MST clustering. We claim that for any other clustering $\mathbf{C} = \{C_1, \dots, C_k\}$,

$$\operatorname{mindist}(\mathbf{C}) \leq \operatorname{mindist}(\mathbf{C}^*) \quad (24)$$

Assume that this was not the case, so $\operatorname{mindist}(\mathbf{C}) > \operatorname{mindist}(\mathbf{C}^*)$ and therefore there exists a $p, q \in C_i, C_j$ such that $d(p, q) = \operatorname{mindist}(\mathbf{C}) > \operatorname{mindist}(\mathbf{C}^*)$. Since this is a different clustering, p, q must have been in the same cluster C_i^* . But note that since Kruskal adds edges in increasing length, all edges within a cluster must have length less edges that go across two clusters.



So $d(p, q)$ must be the less than the length of all edges within a cluster in \mathbf{C}^* . But all within-cluster edges must be smaller than $\operatorname{mindist}(\mathbf{C}^*)$, meaning that $\operatorname{mindist}(\mathbf{C}^*) > d(p, q)$, contradicting the fact that is is greater, and we are done.

If you define the distance between two clusters to be the distance between the centroids (mean point), then this is called *average linkage* (min avg distance). If we define the cluster distance as the maximum distance between two points, then it is called *complete linkage* (min max distance). Kruskal's algorithm only worked for the single linkage case but may not work for these additional definitions. This is why there is usually a whole suite of clustering algorithms for a particular problem and we just find out which one fits the data the best. Furthermore, we have done *bottom-up clustering*, where we took individual points to make clusters. In *top-down clustering*, we take the whole set and cut it up into clusters.

Algorithm 6.15 (Traveling Salesman Problem (TSP))

It's not like finding a tree, but we want to find a path that visits everything.

Algorithm 3

Require:

- 1:
 - 2: **function** TSP(x)
 - 3: **end function**
-

7 Greedy Algorithms

Greedy algorithms are easy to implement and easy to conceptualize, but they are often not correct. So the only interest in them is proving if they are correct. We have done greedy algorithms like Dijkstra and finding MSTs. Every step, greedy algorithms make an irrevocable decision of what to do and cannot undo it.

8 Linear Programming