

1 Introduction

In general, when analyzing an algorithm, we want to know two things.

1. Does it work?
2. Does it have good performance?

Today, we'll begin to see how we might formally answer these questions, through the lens of sorting. We'll start, as a warm-up, with INSERTIONSORT, and then move on to the (more complicated) MERGESORT. MERGESORT will also allow us to continue our exploration of *Divide and Conquer*.

2 InsertionSort

In your pre-lecture exercise, you should have taken a look at a couple of ways of implementing INSERTIONSORT. Here's one:

```
def InsertionSort(A):
    for i in range(1, len(A)):
        current = A[i]
        j = i - 1
        while j >= 0 and A[j] > current:
            A[j + 1] = A[j]
            j -= 1
        A[j + 1] = current
```

Let us ask our two questions: does this algorithm work, and does it have good performance?

2.1 Correctness of InsertionSort

Once you figure out what INSERTIONSORT is doing (see the slides for the intuition on this), you may think that it's "obviously" correct. However, if you didn't know what it was doing and just got the above code, maybe this wouldn't be so obvious. Additionally, for algorithms that we'll study in the future, it *won't* always be obvious that it works, and so we'll have to prove it. To warm us up for those proofs, let's carefully go through a proof of correctness of INSERTIONSORT.

We'll do the proof by maintaining a *loop invariant*, in this case that after iteration i , then $A[:i+1]$ is sorted. This is obviously true when $i = 0$ (because the empty list $A[:1] = []$ is definitely sorted) and then we'll show that for any $i > 0$, if it's true for $i - 1$, then it's true for i . At the end of the day, we'll conclude that $A[:n]$ (aka, the whole thing) is sorted and we'll be done.

Formally, we will proceed by induction.

- **Inductive hypothesis.** After iteration i of the outer loop, $A[:i+1]$ is sorted.
- **Base case.** When $i = 0$, $A[:1]$ contains only one element, and this is sorted.

- **Inductive step.** Suppose that the inductive hypothesis holds for $i - 1$, so $A[:i]$ is sorted after the $i - 1$ 'st iteration. We want to show that $A[:i+1]$ is sorted after the i 'th iteration.

Suppose that j^* is the largest integer in $\{0, \dots, i - 1\}$ so that $A[j^*] < A[i]$. Then the effect of the inner loop is to turn

$$[A[0], A[1], \dots, A[j^*], \dots, A[i - 1], A[i]]$$

into

$$[A[0], A[1], \dots, A[j^*], A[i], A[j^* + 1], \dots, A[i - 1]].$$

We claim that this latter list is sorted. This is because $A[i] > A[j^*]$, and by the inductive hypothesis, we have $A[j^*] \geq A[j]$ for all $j \leq j^*$, and so $A[i]$ is larger than everything that is positioned before it. Similarly, by the choice of j^* we have $A[i] \leq A[j^* + 1] \leq A[j]$ for all $j \geq j^* + 1$, so $A[i]$ is smaller than everything that comes after it. Thus, $A[i]$ is in the right place. All of the other elements were already in the right place, so this proves the claim.

Thus, after the i 'th iteration completes, $A[:i+1]$ is sorted, and this establishes the inductive hypothesis for i .

- **Conclusion.** By induction, we conclude that the inductive hypothesis holds for all $i \leq n - 1$. In particular, this implies that after the end of the $n - 1$ 'st iteration (after the algorithm ends) $A[:n]$ is sorted. Since $A[:n]$ is the whole list, this means the whole list is sorted when the algorithm terminates, which is what we were trying to show.

The above proof was maybe a bit pedantic: we used a lot of words to prove something that may have been pretty obvious. However, it's important to understand the structure of this argument, because we'll use it a lot, sometimes for more complicated algorithms.

2.2 Running time of InsertionSort

The running time of InsertionSort is about n^2 operations. To be a bit more precise, at iteration i , the algorithm may have to look through and move i elements, so that's about $\sum_{i=1}^n i = \frac{n(n+1)}{2}$ operations.

We're not going to stress the precise operation count, because we'll argue that the end of the lecture that we don't care too much about it. The main question that we have, is, can we do *asymptotically better* than n^2 ? That is, can we come up with an algorithm that sorts an arbitrary list of n integers in time that scales less than n^2 ? For example, like $n^{1.5}$, or $n \log(n)$, or even n ? Next we'll see that MERGESORT will scale like $n \log(n)$, which is much faster.

3 MergeSort

Recall the *Divide-and-conquer* paradigm from the first lecture. In this paradigm, we use the following strategy:

- Break the problem into sub-problems.
- Solve the sub-problems (often recursively)
- Combine the results of the sub-problems to solve the big problem.

At some point, the sub-problems become small enough that they are easy to solve, and then we can stop recursing.

With this approach in mind, MERGESORT is a very natural algorithm to solve the sorting problem. The pseudocode is below:

```

MergeSort(A):
    n = len(A)
    if n <= 1:
        return A
    L = MergeSort( A[:n/2] )
    R = MergeSort( A[n/2:] )
    return Merge(L, R)

```

Above, we are using Python notation, so $A[:n/2] = [A[0], A[1], \dots, A[n/2-1]]$ and $A[n/2:] = [A[n/2], \dots, A[n/2+1]]$. Additionally, we're using integer division, so $n/2$ means $\lfloor n/2 \rfloor$.

How do we do the **Merge** procedure? We need to take two sorted arrays, L and R , and merge them into a sorted array that contains both of their elements. See the slides for a walkthrough of this procedure.

```

Merge(L, R):
    m = len(L) + len(R)
    S = [ ]
    for k in range(m):
        if L[i] < R[j]:
            S.append( L[i] )
            i += 1
        else:
            S.append( R[j] )
            j += 1
    return S

```

Note: This pseudocode is incomplete! What happens if we get to the end of L or R ? Try to adapt the pseudocode above to fix this (or check out the IPython notebook for working Python code).

As before, we need to ask: Does it work? And does it have good performance?

3.1 Correctness of MergeSort

Let's focus on the first question first. As before, we'll proceed by induction. This time, we'll maintain a *recursion invariant* that any time MERGESORT returns, it returns a sorted array.

- **Inductive Hypothesis.** Whenever MERGESORT returns an array of size $\leq i$, that array is sorted.
- **Base case.** Suppose that $i = 1$. Then whenever MERGESORT returns an array of length 0 or length 1, that array is sorted. (Since all array of length 0 and 1 are sorted). So the Inductive Hypothesis holds for $i = 1$.
- **Inductive step.** We need to show that if MERGESORT always returns a sorted array on inputs of length $\leq i - 1$, then it always does for length $\leq i$. Suppose that MERGESORT has an input of length i . Then L and R are both of length $\leq i - 1$, so by induction, L and R are both sorted. Thus, the inductive step boils down to the statement:

“When MERGE takes as inputs two sorted arrays L and R , then it returns a sorted array containing all of the elements of L , along with all of the elements of R .”

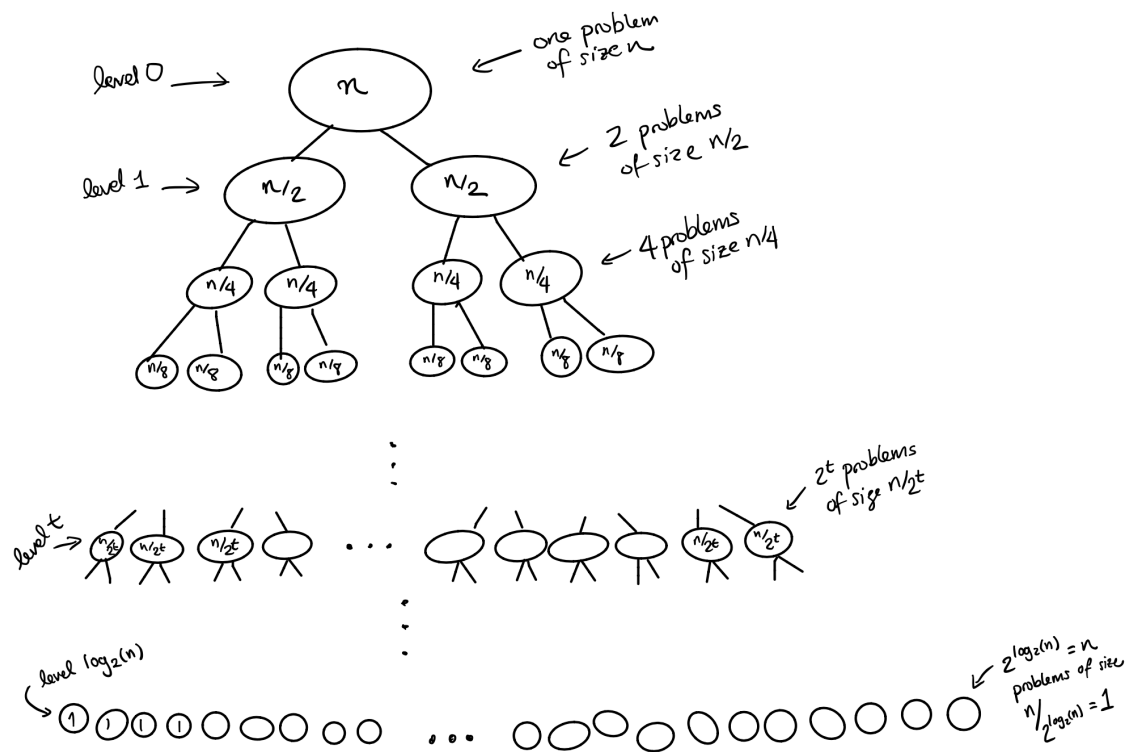
This statement is intuitively true, although proving it rigorously takes a bit of bookkeeping. In fact, it takes another proof by induction! Check out CLRS Section 2.3.1 for a rigorous treatment.

- **Conclusion.** By induction, the Inductive hypothesis holds for all i . In particular, given an array of any length n , MERGESORT returns a sorted version of that array.

3.2 Running time of MergeSort

Finally, we get to our first question in this lecture where the answer may not be intuitively obvious. What is the running time of MergeSort? In the next few lectures, we'll see a few principled ways of analyzing the runtime of a recursive algorithm. Here, we'll just go through one of the ways, which is called the *recursion tree* method.

The idea is to draw a tree representing the computation (see the slides for the visuals). Each node in the tree represents a subproblem, and its children represent the subproblems we need to solve to solve the big sub-problem. The recursion tree for MergeSort looks something like this:



At the top (zeroth) level is the whole problem, which has size n . This gets broken into two sub-problems, each of size $n/2$, and so on. At the t 'th level, there are 2^t problems, each of size $n/2^t$. This continues until we have n problems of size 1, which happens at the $\log(n)$ 'th level.

Some notes:

- In this class, logarithms will **always** be base 2, unless otherwise noted.
- We are being a bit sloppy in the picture above: what if n is not a power of 2? Then $n/2^j$ might not be an integer. In the pseudocode above, we actually break a problem of size n into problems of size $\lfloor n/2 \rfloor$ and $\lceil n/2 \rceil$. Keeping track of this in our analysis will be messy, and it won't add much, so we will ignore it, and for now we will assume that n is a power of 2.¹

¹To formally justify the assumption that n is a power of 2, notice that we can always sort a *longer* list of length $n' = 2^{\lceil \log_2(n) \rceil}$. That is, we'll add extra entries, whose values are ∞ , to the list. Then we sort the new list of length n' , and return the first n values. Since $n' \leq 2n$ (why?) this won't affect the asymptotic running time. Also see CLRS Section 4.6.2 for a rigorous analysis of the original algorithm with floors and ceilings.

In order to figure out the total amount of work, we will figure out how much work is done at each node in the tree, and add it all up. To that end, we tally up the work that is done in a particular node in the tree—that is, in a particular call to MERGESORT. There are three things:

1. Checking the base case
2. Making recursive calls (but we don't count the work actually done in those recursive calls; that will count in other nodes)
3. Running MERGE.

Let's analyze each of these. Suppose that our input has size m (so that $m = n/2^j$ for some j).

1. Checking the base case doesn't take much time. For concreteness, let us say that it takes one operation to retrieve the length of A , and other operation to compare this length to 1, for a total of two operations.²
2. Making the recursive calls should also be fast. If we implemented the pseudocode well, it should also take a constant number of operations.

Aside: This is a good point to talk about how we interpret pseudocode in this class. Above, we've written `MergeSort(A[:n/2])` as an example of a recursive call. This makes it clear that we are supposed to recurse on the first half of the list, but it's not clear how we actually implement that. Our "pseudocode" above is in fact working Python code, and in Python, this implementation, while clear, is a bit inefficient. That is, written this way, Python will actually *copy* the first $n/2$ elements of the list before sending them to the recursive call. A much better way would be to instead just pass in pointers to the 0'th and $n/2 - 1$ 'st index in the list. This would result in a faster algorithm, but kludgier pseudocode. In this class, we generally will opt for cleaner pseudocode, as long as it does not hurt the *asymptotic* running time of the algorithm. In this case, our simple-but-slower pseudocode turns out not to affect the asymptotic running time, so we'll stick with this.

In light of the above **Aside**, let's suppose that this step takes $m + 2$ operations, $m/2$ to copy each half of the list over, and 2 operations to store the results. Of course, a better implementation of this step would only take a constant number (say, four) operations.

3. The third thing is the tricky part. We claim that the MERGE step also takes about m operations.

Consider a single call to MERGE, where we'll assume the total size of A is m numbers. How long will it take for MERGE to execute? To start, there are two initializations for i and j . Then, we enter a for loop which will execute m times. Each loop will require one comparison, followed by an assignment to S and an increment of i or j . Finally, we'll need to increment the counter in the for loop k . If we assume that each operation costs us a certain amount of time, say $Cost_a$ for assignment, $Cost_c$ for comparison, $Cost_i$ for incrementing a counter, then we can express the total time of the MERGE subroutine as follows:

$$2Cost_a + m(Cost_a + Cost_c + 2Cost_i)$$

This is a precise, but somewhat unruly expression for the running time. In particular, it seems difficult to keep track of lots of different constants, and it isn't clear which costs will be more or less expensive (especially if we switch programming languages or machine architectures). To simplify our analysis, we choose to assume that there is some global constant c_{op} which represents the cost of an operation. You may think of c_{op} as $\max\{Cost_a, Cost_c, Cost_i, \dots\}$. We can then bound the amount of running time for MERGE as

$$2c_{op} + 4c_{op}m = 2 + 4m \text{ operations}$$

²Of course, there's no reason that the "operation" of getting the length of A should take the same amount of time as the "operation" of comparing two integers. This disconnect is one of the reasons we'll introduce big-Oh notation at the end of this lecture.

Thus, the total number of operations is at *most*

$$2 + (m + 2) + 4m + 2 \leq 11m$$

using the assumption that $m \geq 1$. This is a very loose bound; for larger m this will be much closer to $5m$ than it is to $11m$. But, as we'll discuss more below, the difference between 5 and 11 won't matter too much to us, so much as the linear dependence on m .

Now that we understand how much work is going on in one call where the input has size m , let's add it all up to obtain a bound on the number of operations required for MERGESORT. In a MERGE of m numbers, we want to translate this into a bound on the number of operations required for MERGESORT. At first glance, the pessimist in you may be concerned that at each level of recursive calls, we're spawning an exponentially increasing number of copies of MERGESORT (because the number of calls at each depth doubles). Dual to this, the optimist in you will notice that at each level, the inputs to the problems are decreasing at an exponential rate (because the input size halves with each recursive call). Today, the optimists win out.

Claim 1. MERGESORT *requires at most $11n \log n + 11n$ operations to sort n numbers.*

Before we go about proving this bound, let's first consider whether this running time bound is good. We mentioned earlier that more obvious methods of sorting, like INSERTIONSORT, required roughly n^2 operations. How does $n^2 = n \cdot n$ compare to $n \cdot \log n$? An intuitive definition of $\log n$ is the following: "Enter n into your calculator. Divide by 2 until the total is ≤ 1 . The number of times you divided is the logarithm of n ." This number in general will be significantly smaller than n . In particular, if $n = 32$, then $\log n = 5$; if $n = 1024$, then $\log n = 10$. Already, to sort arrays of $\approx 10^3$ numbers, the savings of $n \log n$ as compared to n^2 will be orders of magnitude. At larger problem instances of 10^6 , 10^9 , etc. the difference will become even more pronounced! $n \log n$ is much closer to growing linearly (with n) than it is to growing quadratically (with n^2).

One way to argue about the running time of recursive algorithms is to use *recurrence relations*. A recurrence relation for a running time expresses the time it takes to solve an input of size n in terms of the time required to solve the recursive calls the algorithm makes. In particular, we can write the running time $T(n)$ for MERGESORT on an array of n numbers as the following expression.

$$\begin{aligned} T(n) &= T(n/2) + T(n/2) + T(\text{MERGE}(n)) \\ &\leq 2 \cdot T(n/2) + 11n \end{aligned}$$

There are a number of sophisticated and powerful techniques for solving recurrences. We will cover many of these techniques in the coming lectures. Today, we can actually analyze the running time directly.

Proof of Claim 1. Consider the recursion tree of a call to MERGESORT on an array of n numbers. Assume for simplicity that n is a power of 2. Let's refer to the initial call as Level 0, the proceeding recursive calls as Level 1, and so on, numbering the level of recursion by its depth in the tree. How deep is the tree? At each level, the size of the inputs is divided in half, and there are no recursive calls when the input size is ≤ 1 element. By our earlier "definition", this means the bottom level will be Level $\log n$. Thus, there will be a total of $\log n + 1$ levels.

We can now ask two questions: (1) How many subproblems are there at Level i ? (2) How large are the individual subproblems at Level i ? We can observe that at the i th level, there will be 2^i subproblems, each with inputs of size $n/2^i$.

We've already worked out that each sub-problem with input of size $n/2^i$ takes at most $11n/2^i$ operations. Now we can add this up:

$$\begin{aligned} \text{Work at Level } i &= (\text{number of subproblems}) \cdot (\text{work per subproblem}) \\ &\leq 2^i \cdot 11 \left(\frac{n}{2^i} \right) \\ &= 11n \text{ operations.} \end{aligned}$$

Importantly, we can see that the work done at Level i is independent of i – it only depends on n and is the same for every level. This means we can bound the total running time as follows:

$$\begin{aligned}\text{Total number of operations} &= (\text{operations per level}) \cdot (\text{number of levels}) \\ &\leq (11n) \cdot (\log n + 1) \\ &= 11n \log n + 11n\end{aligned}$$

□

This proves the claim, and we’re done!

4 Guiding Principles for Algorithm Design and Analysis

After going through the algorithm and analysis, it is natural to wonder if we’ve been too sloppy. In particular, note that the algorithm never “looks at” the input. For instance, what if we received the sequence of numbers $[1, 2, 3, 5, 4, 6, 7, 8]$? Clearly, there is a “sorting algorithm” for this sequence that only takes a few operations, but MERGESORT runs through all $\log n + 1$ levels of recursion anyway. Would it be better to try to design our algorithms with this in mind? Additionally, in our analysis, we’ve given a very loose upper bound on the time required of MERGE and dropped a number of constant factors and lower order terms. Is this a problem? In what follows, we’ll argue that these are actually *features*, not bugs, in the design and analysis of the algorithm.

4.1 Worst-Case Analysis

One guiding principle we’ll use throughout the class is that of *Worst-Case Analysis*. In particular, this means that we want any statement we make about our algorithms to hold for *every* possible input. Stated differently, we can think about playing a game against an adversary, who wants to maximize our running time (make it as bad as possible). We get to specify an algorithm and state a running time $T(n)$; the adversary then chooses an input. We win the game if even in the worst case, whatever input the adversary chooses (of size n), our algorithm runs in at most $T(n)$ time.

Note that because our algorithm made no assumptions about the input, then our running time bound will hold for every possible input. This is a very strong, robust guarantee.³

4.2 Asymptotic Analysis

Throughout our argument about MERGESORT, we combined constants (think $Cost_a, Cost_i$, etc.) and gave very loose upper bounds (like being okay with a naive implementation of our pseudocode, or with this very wasteful upper bound $11m$ on the work done at a subproblem in MERGESORT). Why did we choose to do this? First, it makes the math much easier. But does it come at the cost of getting the “right” answer? Would we get a more predictive result if we threw all these exact expressions back into the analysis? From the perspective of an algorithm designer, the answer to both of these questions is a resounding “No”. As an algorithm designer, we want to come up with results that are broadly applicable, whose truth does not depend on features of a specific programming language or machine architecture. The constants that we’ve dropped will depend greatly on the language and machine on which you’re working. For the same reason we use pseudocode instead of writing our algorithms in Java, trying to quantify the exact running time of an algorithm would be inappropriately specific. This is not to say that constant factors never matter in applications (e.g. I would be rather upset if my web browser ran 7 times slower than it does now) but worrying about these factors is not the goal of this class. In this class, our goal will be to argue about which strategies for solving problems are wise and why.

³In the case where you have significant domain knowledge about which inputs are likely, you may choose to design an algorithm that works well in expectation on these inputs (this is frequently referred to as Average-Case Analysis). This type of analysis is often much more tricky, and requires strong assumptions on the input.

In particular, we will focus on *Asymptotic Analysis*. This type of analysis focuses on the running time of your algorithm as your input size gets very large (i.e. $n \rightarrow +\infty$). This framework is motivated by the fact that if we need to solve a small problem, it doesn't cost that much to solve it by brute-force. If we want to solve a large problem, we may need to be much more creative in order for the problem to run efficiently. From this perspective, it should be very clear that $11n(\log n + 1)$ is much better than $n^2/2$. (If you are unconvinced, try plugging in some values for n .)

Intuitively, we'll say that an algorithm is "fast" when the running time grows "slowly" with the input size. In this class, we want to think of growing "slowly" as growing as close to linear as possible. Based on this intuitive notion, we can come up with a formal system for analyzing how quickly the running time of an algorithm grows with its input size.

4.3 Asymptotic Notation

To talk about the running time of algorithms, we will use the following notation. $T(n)$ denotes the runtime of an algorithm on input of size n .

"Big-Oh" Notation:

Intuitively, Big-Oh notation gives an upper bound on a function. We say $T(n)$ is $O(f(n))$ when as n gets big, $f(n)$ grows at least as quickly as $T(n)$. Formally, we say

$$T(n) = O(f(n)) \iff \exists c, n_0 > 0 \text{ s.t. } \forall n \geq n_0, 0 \leq T(n) \leq c \cdot f(n)$$

"Big-Omega" Notation:

Intuitively, Big-Omega notation gives a lower bound on a function. We say $T(n)$ is $\Omega(f(n))$ when as n gets big, $f(n)$ grows at least as slowly as $T(n)$. Formally, we say

$$T(n) = \Omega(f(n)) \iff \exists c, n_0 > 0 \text{ s.t. } \forall n \geq n_0, 0 \leq c \cdot f(n) \leq T(n)$$

"Big-Theta" Notation:

$T(n)$ is $\Theta(f(n))$ if and only if $T(n) = O(f(n))$ and $T(n) = \Omega(f(n))$. Equivalently, we can say that

$$T(n) = \Theta(f(n)) \iff \exists c_1, c_2, n_0 > 0 \text{ s.t. } \forall n \geq n_0, 0 \leq c_1 f(n) \leq T(n) \leq c_2 f(n)$$

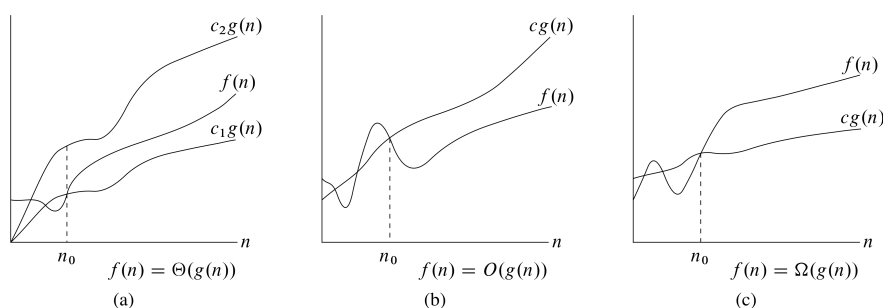


Figure 3.1 from CLRS – Examples of Asymptotic Bounds

(Note: In these examples $f(n)$ corresponds to our $T(n)$ and $g(n)$ corresponds to our $f(n)$.)

We can see that these notations really do capture exactly the behavior that we want – namely, to focus on the rate of growth of a function as the inputs get large, ignoring constant factors and lower order terms. As a sanity check, consider the following example and non-example.

Claim 2. All degree- k polynomials⁴ are $O(n^k)$.

Proof of Claim. Suppose $T(n)$ is a degree- k polynomial. That is, $T(n) = a_k n^k + \dots + a_1 n + a_0$ for some choice of a_i 's where $a_k \neq 0$. To show that $T(n)$ is $O(n^k)$ we must find a c and n_0 such that for all $n \geq n_0$ $T(n) \leq c \cdot n^k$. (Since $T(n)$ represents the running time of an algorithm, we assume it is positive.) Let $n_0 = 1$ and let $a^* = \max_i |a_i|$. We can bound $T(n)$ as follows:

$$\begin{aligned} T(n) &= a_k n^k + \dots + a_1 n + a_0 \\ &\leq a^* n^k + \dots + a^* n + a^* \\ &\leq a^* n^k + \dots + a^* n^k + a^* n^k \\ &= (k+1)a^* \cdot n^k \end{aligned}$$

Let $c = (k+1)a^*$ which is a constant, independent of n . Thus, we've exhibited c, n_0 which satisfy the Big-Oh definition, so $T(n) = O(n^k)$. \square

Claim 3. For any $k \geq 1$, n^k is not $O(n^{k-1})$.

Proof of Claim. By contradiction. Assume $n^k = O(n^{k-1})$. Then there is some choice of c and n_0 such that $n^k \leq c \cdot n^{k-1}$ for all $n \geq n_0$. But this in turn means that $n \leq c$ for all $n \geq n_0$, which contradicts the fact that c is a constant, independent of n . Thus, our original assumption was false and n^k is not $O(n^{k-1})$. \square

⁴To be more precise, all degree- k polynomials T so that $T(n) \geq 0$ for all $n \geq 1$. How would you adapt this proof to be true for all degree- k polynomials T with a positive leading coefficient?

1 Introduction

Last lecture, we covered the master theorem, which can be used for recurrences of a certain form. Recall that if we have a recurrence $T(n) = a \cdot T\left(\frac{n}{b}\right) + O(n^d)$ where $a \geq 1, b > 1$, then

$$T(n) = \begin{cases} O(n^d \log n) & \text{if } a = b^d \\ O(n^d) & \text{if } a < b^d \\ O(n^{\log_b a}) & \text{if } a > b^d \end{cases}$$

Many algorithms that result from the divide-and-conquer paradigm yield recurrence relations for their run-times that have the above form—namely algorithms that divide the problem into *equal*-sized sub-pieces at each recursion.

Today, we will introduce a problem where the master theorem cannot be applied: the problem of finding the k th smallest element in an unsorted array. First, we show it can be done in $O(n \log n)$ time via sorting and that any correct algorithm must run in $\Omega(n)$ time. However, it is not obvious that a linear-time selection algorithm exists. We present a linear-time selection algorithm, with an intuition for why it has the desired properties to achieve $O(n)$ running time. The two high-level goals of this lecture are 1) to cover a really cool and surprising algorithm, and 2) illustrate that some divide-and-conquer algorithms yield recurrence relations that cannot be analyzed via the “Master Method/Theorem”, yet one can (often) still successfully analyze them.

2 Selection

The selection problem is to find the k th smallest number in an array A .

Input: array A of n numbers, and an integer $k \in \{1, \dots, n\}$.

Output: the k -th smallest number in A .

One approach is to sort the numbers in ascending order, and then return the k th number in the sorted list. This takes $O(n \log n)$ time, since it takes $O(n \log n)$ time for the sort (e.g. by MergeSort) and $O(1)$ time to return k th number.

2.1 Minimum Element

As always, we ask if we can do better (i.e. faster in big-O terms). In the special case where $k = 1$, selection is the problem of finding the minimum element. We can do this in $O(n)$ time by scanning through the array and keeping track of the minimum element so far. If the current element is smaller than the minimum so far, we update the minimum.

In fact, this is the best running time we could hope for.

Definition 2.1. A *deterministic algorithm* is one which, given a fixed input, always performs the same operations (as opposed to an algorithm which uses randomness).

Claim 1. Any deterministic algorithm for finding the minimum has runtime $\Omega(n)$.

Algorithm 1: SELECTMIN(A)

```
 $m \leftarrow \infty;$ 
 $n \leftarrow \text{length}(A);$ 
for  $i = 1$  to  $n$  do
    if  $A(i) < m$  then
         $m \leftarrow A(i);$ 
return  $m;$ 
```

Proof of Claim 1. Intuitively, the claim holds because any algorithm for the minimum must look at all the elements, each of which could be the minimum. Suppose a correct deterministic algorithm does not look at $A(i)$ for some i . Then the output cannot depend on $A(i)$, so the algorithm returns the same value whether $A(i)$ is the minimum element or the maximum element. Therefore the algorithm is not always correct, which is a contradiction. So there is no sublinear deterministic algorithm for finding the minimum. \square

So for $k = 1$, we have an algorithm which achieves the best running time possible. By similar reasoning, this lower bound of $\Omega(n)$ applies to the general selection problem. So ideally we would like to have a linear-time selection algorithm in the general case.

3 Linear-Time Selection

In fact, a linear-time selection algorithm does exist. Before showing the linear time selection algorithm, it's helpful to build some intuition on how to approach the problem. The high-level idea will be to try to do a Binary Search over an unsorted input. At each step, we hope to divide the input into two parts, the subset of smaller elements of A , and the subset of larger elements of A . We will then determine whether the k th smallest element lies in the first part (with the “smaller” elements) or the part with larger elements, and recurse on exactly one of those two parts.

How do we decide how to partition the array into these two pieces? Suppose we have a black-box algorithm CHOOSEPIVOT that chooses some element in the array A , and we use this pivot to define the two sets—any $A[i]$ less than the pivot is in the set of “smaller” values, and any $A[i]$ greater than the pivot is in the other part. We will figure out precisely how to specify this subroutine ChoosePivot a bit later, after specifying the high-level algorithm structure. For clarity we'll assume all elements are distinct from now on, but the idea generalizes easily. Let n be the size of the array and assume we are trying to find the k^{th} element.

Algorithm 2: SELECT(A, n, k)

```
if  $n == 1$  then
     $\text{return } A[1];$ 
 $p \leftarrow \text{CHOOSEPIVOT}(A, n);$ 
 $A_{<} \leftarrow \{A(i) \mid A(i) < p\};$ 
 $A_{>} \leftarrow \{A(i) \mid A(i) > p\};$ 
if  $|A_{<}| = k - 1$  then
     $\text{return } p;$ 
else if  $|A_{<}| > k - 1$  then
     $\text{return SELECT}(A_{<}, |A_{<}|, k);$ 
else if  $|A_{<}| < k - 1$  then
     $\text{return SELECT}(A_{>}, |A_{>}|, k - |A_{<}| - 1);$ 
```

At each iteration, we use the element p to partition the array into two parts: all elements smaller than the pivot and all elements larger than the pivot, which we denote $A_{<}$ and $A_{>}$, respectively.

Depending on what the size of the resulting sub-arrays are, the runtime can be different. For example, if one of these sub-arrays is of size $n - 1$, at each iteration, we only decreased the size of the problem by 1, resulting in total running time $O(n^2)$. If the array is split into two equal parts, then the size of the problem at iteration reduces by half, resulting in a linear time solution. (We assume CHOOSEPIVOT runs in $O(n)$.)

Claim 2. *If the pivot p is chosen to be the minimum or maximum element, then SELECT runs in $\Theta(n^2)$ time.*

Proof. At each iteration, the number of elements decreases by 1. Since running CHOOSEPIVOT and creating $A_{<}$ and $A_{>}$ takes linear time, the recurrence for the runtime is $T(n) = T(n - 1) + \Theta(n)$. Expanding this,

$$T(n) \leq c_1n + c_1(n - 1) + c_1(n - 2) + \dots + c_1 = c_1n(n + 1)/2$$

and

$$T(n) \geq c_2n + c_2(n - 1) + c_2(n - 2) + \dots + c_2 = c_2n(n + 1)/2.$$

We conclude that $T(n) = \Theta(n^2)$. □

Claim 3. *If the pivot p is chosen to be the median element, then SELECT runs in $O(n)$ time.*

Proof. Intuitively, the running time is linear since we remove half of the elements from consideration each iteration. Formally, each recursive call is made on inputs of half the size, namely, $T(n) \leq T(n/2) + cn$. Expanding this, the runtime is $T(n) \leq cn + cn/2 + cn/4 + \dots + c \leq 2cn$, which is $O(n)$. □

So how do we design CHOOSEPIVOT that chooses a pivot in linear time? In the following, we describe three ideas.

3.1 Idea #1: Choose a random pivot

As we saw earlier, depending on the pivot chosen, the worst-case runtime can be $O(n^2)$ if we are unlucky in the choice of the pivot at every iteration. As you might expect, it is extremely unlikely to be this unlucky, and one can prove that the *expected* runtime is $O(n)$ provided the pivot is chosen uniformly at random from the set of elements of A . In practice, this randomized algorithm is what is implemented, and the hidden constant in the $O(n)$ runtime is very small. We cover the rather clever analysis of this randomized algorithm in CS265 (“Randomized Algorithms and Probabilistic Analysis”). . . .

3.2 Idea #2: Choose a pivot that create the most “balanced” split

Consider CHOOSEPIVOT that returns the pivot that creates the most “balanced” split, which would be the median of the array. However, this is exactly selection problem we are trying to solve, with $k = n/2$! As long as we do not know how to find the median in linear time, we cannot use this procedure as CHOOSEPIVOT.

3.3 Idea #3: Find a pivot “close enough” to the median

Given a linear-time median algorithm, we can solve the selection problem in linear time (and vice versa). Although ideally we would want to find the median, notice that as far as correctness goes, there was nothing special about partitioning around the median. We could use this same idea of partitioning and recursing on a smaller problem even if we partition around an arbitrary element. To get a good runtime, however, we need to guarantee that the subproblems get smaller quickly. In 1973, Blum, Floyd, Pratt, Rivest, and Tarjan came up with the Median of Medians algorithm. It is similar to the previous algorithm, but rather than partitioning around the exact median, uses a surrogate “median of medians”. We update CHOOSEPIVOT accordingly.

What is this algorithm doing? First it divides A into segments of size 5. Within each group, it finds the median by first sorting the elements with MERGESORT. Recall that MERGESORT sorts in $O(n \log n)$ time. However, since each group has a constant number of elements, it takes constant time to sort. Then it makes a

Algorithm 3: CHOOSEPIVOT(A, n)

```
Split  $A$  into  $g = \lceil n/5 \rceil$  groups  $p_1, \dots, p_g$ ;  
for  $i = 1$  to  $g$  do  
   $p_i \leftarrow \text{MERGESORT}(p_i)$ ;  
 $C \leftarrow \{\text{median of } p_i \mid i = 1, \dots, g\}$ ;  
 $p \leftarrow \text{SELECT}(C, g, g/2)$ ;  
return  $p$ ;
```

recursive call to SELECT to find the median of C , the median of medians. Intuitively, by partitioning around this value, we are able to find something that is close to the true median for partitioning, yet is ‘easier’ to compute, because it is the median of $g = \lceil n/5 \rceil$ elements rather than n . The last part is as before: once we have our pivot element p , we split the array and recurse on the proper subproblem, or halt if we found our answer.

We have devised a slightly complicated method to determine which element to partition around, but the algorithm remains correct for the same reasons as before. So what is its running time? As before, we’re going to show this by examining the size of the recursive subproblems. As it turns out, by taking the median of medians approach, we have a guarantee on how much smaller the problem gets each iteration. The guarantee is good enough to achieve $O(n)$ runtime.

3.3.1 Running Time

Lemma 3.1. $|A_{<}| \leq 7n/10 + 5$ and $|A_{>}| \leq 7n/10 + 5$.

Proof of Lemma 3.1. p is the median of p_1, \dots, p_g . Because p is the median of $g = \lceil n/5 \rceil$ elements, the medians of $\lceil g/2 \rceil - 1$ groups p_i are smaller than p . If p is larger than a group median, it is larger than at least three elements in that group (the median and the smaller two numbers). This applies to all groups except the remainder group, which might have fewer than 5 elements. Accounting for the remainder group, p is greater than at least $3 \cdot (\lceil g/2 \rceil - 2)$ elements of A . By symmetry, p is less than at least the same number of elements.

Now,

$$\begin{aligned} |A_{>}| &= \# \text{ of elements greater than } p \\ &\leq (n - 1) - 3 \cdot (\lceil g/2 \rceil - 2) \\ &= n + 5 - 3 \cdot \lceil g/2 \rceil \\ &\leq n - 3n/10 + 5 \\ &= 7n/10 + 5. \end{aligned} \tag{1}$$

By symmetry, $|A_{<}| \leq 7n/10 + 5$ as well.

Intuitively, we know that 60% of half of the groups are less than the pivot, which is 30% of the total number of elements, n . Therefore, at most 70% of the elements are greater than the pivot. Hence, $|A_{>}| \approx 7n/10$. We can make the same argument for $|A_{<}|$. \square

The recursive call used to find the median of medians has input of size $\lceil n/5 \rceil \leq n/5 + 1$. The other work in the algorithm takes linear time: constant time on each of $\lceil n/5 \rceil$ groups for MERGESORT (linear time total for that part), $O(n)$ time scanning A to make $A_{<}$ and $A_{>}$.

Thus, we can write the full recurrence for the runtime,

$$T(n) \leq \begin{cases} c_1 n + T(n/5 + 1) + T(7n/10 + 5) & \text{if } n > 5 \\ c_2 & \text{if } n \leq 5. \end{cases}$$

How do we prove that $T(n) = O(n)$? The master theorem does not apply here. Instead, we will prove this using the substitution method.

4 The Substitution Method

Recurrence trees can get quite messy when attempting to solve complex recurrences. With the substitution method, we can guess what the runtime is, plug it in to the recurrence and see if it works out.

Given a recurrence $T(n) \leq cf(n) + \sum_{i=1}^k T(n_i)$, we can guess that the solution to the recurrence is

$$T(n) \leq \begin{cases} d \cdot g(n_0) & \text{if } n = n_0 \\ d \cdot g(n) & \text{if } n > n_0 \end{cases}$$

for some constants $d > 0$ and $n_0 \geq 1$ and a function $g(n)$. We are essentially guessing that $T(n) \leq O(g(n))$.

For our base case we must show that you can pick some d such that $T(n_0) \leq d \cdot g(n_0)$. For example, this can follow from our standard assumption that $T(1) = 1$.

Next we assume that our guess is correct for everything smaller than n , meaning $T(n') \leq d \cdot g(n')$ for all $n' < n$. Using the inductive hypothesis, we prove the guess for n . We must pick some d such that

$$f(n) + \sum_{i=1}^k d \cdot g(n_i) \leq d \cdot g(n), \text{ whenever } n \geq n_0.$$

Typically the way this works is that you first try to prove the inductive step starting from the inductive hypothesis, and then from this obtain a condition that d needs to obey. Using this condition you try to figure out the base case, i.e., what n_0 should be.

4.1 Solving the Recurrence of Select using the Substitution Method

For simplicity, we consider the recurrence $T(n) \leq T(n/5) + T(7n/10) + cn$ instead of the exact recurrence of SELECT.

To prove that $T(n) = O(n)$, we guess:

$$T(n) \leq \begin{cases} dn_0 & \text{if } n = n_0 \\ d \cdot n & \text{if } n > n_0 \end{cases}$$

For the base case, we pick $n_0 = 1$ and use the standard assumption that $T(1) = 1 \leq d$. For the inductive hypothesis, we assume that our guess is correct for any $n < k$, and we prove our guess for k . That is, consider d such that for all $n_0 \leq n < k$, $T(n) \leq dn$.

To prove for $n = k$, we solve the following equation:

$$T(k) \leq T(k/5) + T(7k/10) + ck \leq dk/5 + 7dk/10 + ck \leq dk$$

$$9/10d + c \leq d$$

$$c \leq d/10$$

$$d \geq 10c$$

Therefore, we can choose $d = \max(1, 10c)$, which is a constant factor. The induction is completed. By the definition of big-O, the recurrence runs in $O(n)$ time.

4.2 Issues when using the Substitution Method

Now we will try out an example where our guess is incorrect. Consider the recurrence $T(n) = 2T(\frac{n}{2}) + n$ (similar to MergeSort). We will guess that the algorithm is linear.

$$T(n) \leq \begin{cases} dn_0 & \text{if } n = n_0 \\ d \cdot n & \text{if } n > n_0 \end{cases}$$

We try the inductive step. We try to pick some d such that for all $n \geq n_0$,

$$n + \sum_{i=1}^k dg(n_i) \leq d \cdot g(n)$$

$$n + 2 \cdot d \cdot \frac{n}{2} \leq dn$$

$$n(1 + d) \leq dn$$

$$n + dn \leq dn$$

$$n < 0,$$

However, the above can never be true, and there is no choice of d that works! Thus our guess was incorrect.

This time the guess was incorrect since MergeSort takes superlinear time. Sometimes, however, the guess can be asymptotically correct but the induction might not work out. Consider for instance $T(n) \leq 2T(n/2) + 1$.

We know that the runtime is $O(n)$ so let's try to prove it with the substitution method. Let's guess that $T(n) \leq cn$ for all $n \geq n_0$.

First we do the induction step: We assume that $T(n/2) \leq cn/2$ and consider $T(n)$. We want that $2 \cdot cn/2 + 1 \leq cn$, that is, $cn + 1 \leq cn$. However, this is impossible.

This doesn't mean that $T(n)$ is not $O(n)$, but in this case we chose the wrong linear function. We could guess instead that $T(n) \leq cn - 1$. Now for the induction we get $2 \cdot (cn/2 - 1) + 1 = cn - 1$ which is true for all c . We can then choose the base case $T(1) = 1$.

1 Lower Bounds for Comparison-Based Sorting Algorithms

See link on the course website.

2 Bucket Sort¹

Recall that our sorting lower bounds applied to the class of algorithms that can only evaluate the values being sorted via *comparison queries*, namely via asking whether a given element is greater than, less than, or equal to some other element. For such algorithms, we proved that any correct algorithm (even a randomized one!) will require $\Omega(n \log n)$ such queries on some input. As with any lower-bound that we prove in a restricted model, it is fruitful to ask “is it possible to have an algorithm that does not fall in this class, and hence is not subject to the lowerbound?” For sorting, the answer is “yes”.

We start by looking at a very simple non-comparison-based sorting algorithm called Bucket Sort. Since it is not comparison-based, it is not restricted by the $\Omega(n \log n)$ lower bound for sorting. For a given input of n objects, each with a corresponding key (or value) in the range $\{0, 1, \dots, r - 1\}$, Bucket Sort will sort the objects by their keys:

1. Create an array A of r buckets where each bucket contains a linked list.
2. For each element in the input array with key k , concatenate the element to the end of the linked list $A[k]$.
3. Concatenate all the linked lists: $A[0], \dots, A[r - 1]$.

The algorithm correctly sorts the n elements by their keys because the elements are placed into buckets by key where bucket i (containing elements with key $= i$) will come before bucket j (containing elements with key $= j$) in A for $i < j$. Therefore, when the algorithm concatenates the buckets, all elements with key $= i$ will come before elements with key $= j$.

The worst case run time of bucket sort is $O(n + r)$ since it does $O(1)$ passes over the n input elements and $O(1)$ passes over the r buckets of A .

An important property (which we will use in the next section) is that the algorithm described above is *stable*: If two input elements x, y have the same key, and x appears before y in the input array, x will appear before y in the output.

3 Radix Sort

Radix Sort is another non-comparison-based sorting algorithm that will use Bucket Sort as a subroutine. Assuming that the input array contains L -digit numbers where each digit ranges from 0 to $r - 1$, Radix Sort sorts the array digit-by-digit (or field-by-field for non-numerical inputs). The algorithm works on input array A as follows:

1. For $j = 1, \dots, L$:
2. Bucket Sort A using the j^{th} digit as the key.

¹Note that this may not be the standard name used in CLRS. What we describe here is similar to Counting Sort from CLRS.

Note that we refer to the least significant digit as the first digit. Hence, the algorithm calls Bucket Sort first using the least significant digit as the key, then again using the second least significant digit, until the most significant digit.

We will show that Radix Sort correctly sorts an input list of n numbers via induction on the iterations of the loop. We prove that by the end of the j^{th} iteration, the elements in A are sorted when considering only the j least significant digits of each element.

Base case: Radix Sort correctly sorts the numbers by the first digit as it uses Bucket Sort to sort the numbers using the least significant digit as a key.

Inductive case: By the induction hypothesis, by the end of iteration $j - 1$, the input numbers have been sorted by the $j - 1$ least significant digits.

After we run Bucket Sort on the elements using digit j as the key, the numbers are sorted by their j^{th} digit. Since Bucket Sort is stable, the elements in each bucket keep their original order, and by the induction hypothesis, they are ordered by their $j - 1$ least significant digits. Since the elements are ordered first by their j^{th} digit, and then by their $j - 1$ least significant digits, we conclude that they are ordered by their j least significant digits.

By the end of iteration L , the numbers are in sorted order.

The worst case run time of Radix Sort is $O(L(n + r))$ since we are calling Bucket Sort on n elements with r possible keys once for each digit in the input numbers. If $r = O(n)$ and $L = O(1)$, then this takes $O(n)$ time.

1 Introduction

Today we'll study another sorting algorithm. Quicksort was invented in 1959 by Tony Hoare. You may wonder why we want to study a new sorting algorithm. We have already studied MergeSort, which we showed to perform significantly better than the trivial $O(n^2)$ algorithm. While MergeSort achieves an $O(n \log n)$ worst-case asymptotic bound, in practice, there are a number of implementation details about MergeSort that make it tricky to achieve high performance. Quicksort is an alternative algorithm, which is simpler to implement in practice. Quicksort will also use a divide and conquer strategy but will use randomization to improve the performance of the algorithm in expectation. Java, Unix, and C stdlib all have implementations of Quicksort as one of their built-in sorting routines.

2 Quicksort Overview

As in all sorting algorithms, we start with an array A of n numbers; again we assume without loss of generality that the numbers are distinct. Quicksort is very similar to the Select algorithm we studied last lecture. The description of Quicksort is the following:

- (1) If length of $A \leq 1$: return A (it is trivially sorted).
- (2) Pick some element $x \leftarrow A[i]$. We call x the pivot.
- (3) Split the rest of A into $A_{<}$ (the elements less than x) and $A_{>}$ (the elements greater than x).
- (4) Rearrange A into $[A_{<}, x, A_{>}]$.
- (5) Recurse on $A_{<}, A_{>}$.

Steps 1-3 define a “partition” function on A . The partition function of Quicksort can vary depending on how the pivot is chosen and also on the implementation. Quicksort is often used in practice because we can implement this step in linear time, and with very small constant factors. In addition, the rearrangement (Step 3) can be done in-place, rather than making several copies of the array (as is done in MergeSort). In these notes we will not describe the details of an in-place implementation, but the pseudocode can be found in CLRS.

3 Speculation on the Runtime

The performance of Quicksort depends on which element is chosen as the pivot. Assume that we choose the k^{th} smallest element; then $|A_{<}| = k - 1$, $|A_{>}| = n - k$.

This allows us to write a recurrence; let $T(n)$ be the runtime of Quicksort on an n -element array. We know the partition step takes $O(n)$ time; therefore the recurrence is

$$T(n) \leq cn + T(k - 1) + T(n - k).$$

For the worst pivot choice (the maximum or minimum element in the array), the runtime will resolve to $T(n) = T(n - 1) + O(n) = O(n^2)$.

One way that seems optimal to define the partition function is to pick the *median* as the pivot. In the above recurrence this would mean that $k = \lceil \frac{n}{2} \rceil$. We showed in the previous lecture that the algorithm

Select can find the median element in linear time. Therefore the recurrence becomes $T(n) \leq cn + 2T(\frac{n}{2})$. This is exactly the same recurrence as MergeSort, which means that this algorithm is guaranteed to run in $O(n \log n)$ time.

Unfortunately, the median selection algorithm is not practical; while it runs in linear time, it has much larger constant factors than we would like. To improve it, we will explore some alternative methods for choosing a pivot.

We leave the proof of correctness of Quicksort as an exercise to the reader (a proof by induction is suggested).

3.1 Random Pivot Selection

One method of “defending” against adversarial input is to choose a random element as the pivot. We observe that it is unlikely that the random element will be either the median (best-case) or the maximum or minimum (worst-case). Note that we have a uniform distribution over the n order statistics of the array (that is, for every $1 \leq i \leq n$ we pick the i^{th} -highest element with the same probability $\frac{1}{n}$). However, for the first time, we encounter a randomized algorithm, and the analysis now becomes more complex. How do we analyze a randomized algorithm?

4 Worst-Case Analysis

In this section we will derive a bound on the worst-case running time of Quicksort. If we consider the worst random choice of pivot at each step, the running time will be $\Theta(n^2)$. We are thus interested in what is the running time of Quicksort on average over all possible choices of the pivots. Note that we still consider the running time for a worst-case input, and average only over the random choices of the algorithm (which is different from averaging over all possible inputs). We formalize the idea of averaging over the random choices of the algorithm by considering the running time of the algorithm on an input I as a random variable and bounding the expectation of that random variable.

Claim 1. *For every input array of size n , the expected running time of Quicksort is $O(n \log n)$.*

Recall that a random variable (often abbreviated as RV) is a function that maps every element in the sample space to a real number. In the case of rolling a die, the real number (or value of the point in the sample space) would be the number on the top of the die. Here the sample space is the set of all possible choices of pivots, and an example for a random variable can be the running time of Quicksort on a specific input I .

Denote by z_i the i^{th} element in the sorted array. For each i, j , we define a random variable $X_{i,j}(\sigma)$ to be the number of times z_i and z_j are compared for a given series of pivot choices σ . What are the possible values for $X_{i,j}(\sigma)$? It can be 0 if z_i and z_j are not compared. Note that all comparisons are with the pivot, and that the pivot is not included in the elements of the arrays in the recursive calls. Thus, no two elements are compared twice. Therefore, $X_{i,j}(\sigma) \in \{0, 1\}$.

Our goal is to compute the expected number of comparisons that Quicksort makes. Recall the definition of expectation:

$$E[X] = \sum_{\sigma} P(\sigma) X(\sigma) = \sum_k k P(x = k).$$

An important property of expectation is the linearity of expectation. For any random variables X_1, \dots, X_n :

$$E \left[\sum_{i=1}^n X_i \right] = \sum_{i=1}^n E[X_i].$$

We start with computing the expected value of $X_{i,j}$. These variables are *indicator random variables*,

which take the value 1 if some event happens, and 0 otherwise. The expected value is

$$\begin{aligned} E[X_{i,j}] &= P(X_{i,j} = 1) \cdot 1 + P(X_{i,j} = 0) \cdot 0 \\ &= P(X_{i,j} = 1) \end{aligned}$$

Let $C(\sigma)$ be the total number of comparisons made by Quicksort for a given set of pivot choices σ :

$$C(\sigma) = \sum_{i=1}^n \sum_{j=i+1}^n X_{i,j}(\sigma).$$

We wish to compute $E[C]$ to get the expected number of comparisons made by Quicksort for an input array of size n .

$$\begin{aligned} E[C] &= E \left[\sum_{i=1}^n \sum_{j=i+1}^n X_{i,j}(\sigma) \right] \\ &= \sum_{i=1}^n E \left[\sum_{j=i+1}^n X_{i,j}(\sigma) \right] \\ &= \sum_{i=1}^n \sum_{j=i+1}^n P(z_i, z_j \text{ are compared}) \end{aligned}$$

Now we find $P(z_i, z_j \text{ are compared})$. Note that each element in the array except the pivot is compared to the pivot at each level of the recurrence. To analyze $P(z_i, z_j \text{ are compared})$, we need to examine the portion of the array $[z_i, \dots, z_j]$. After the array is split using a pivot from $[z_i, \dots, z_j]$, z_i and z_j can no longer be compared. Hence, z_i and z_j are compared only when from $[z_i, \dots, z_j]$, either z_i or z_j is the first one picked as the pivot. So,

$$\begin{aligned} P(z_i, z_j \text{ compared}) &= P(z_i \text{ or } z_j \text{ is the first pivot picked from } [z_i, \dots, z_j]) \\ &= \frac{1}{j-i+1} + \frac{1}{j-i+1} \\ &= \frac{2}{j-i+1} \end{aligned}$$

We return to the expected value of C :

$$\begin{aligned} E[C] &= \sum_{i=1}^n \sum_{j=i+1}^n P(z_i, z_j \text{ are compared}) \\ &= \sum_{i=1}^n \sum_{j=i+1}^n \frac{2}{j-i+1} \end{aligned}$$

Note that for a fixed i ,

$$\begin{aligned} \sum_{j=i+1}^n \frac{1}{j-i+1} &= \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{n-i+1} \\ &\leq \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{n} \end{aligned}$$

And using $\sum_{k=2}^n \frac{1}{k} \leq \ln n$, we get that

$$\begin{aligned} E[C] &= E \left[\sum_{i=1}^n \sum_{j=i+1}^n X_{i,j}(\sigma) \right] \\ &= \sum_{i=1}^n \sum_{j=i+1}^n \frac{2}{j-i+1} \\ &\leq 2n \ln n \end{aligned}$$

Thus, the expected number of comparisons made by Quicksort is no greater than $2n \ln n = O(n \log n)$. To complete the proof, we have to show that the running time is dominated by the number of comparisons. Note that in each recursive call to Quicksort on an array of size k , the algorithm performs $k - 1$ comparisons in order to split the array, and the amount of work done is $O(k)$. In addition, Quicksort will be called on single-element arrays at most once for each element in the original array, so the total running time of Quicksort is $O(C + n)$. In conclusion, the expected running time of Quicksort on worst-case input is $O(n \log n)$.

4.1 Alternative Proof

Here we provide an alternative method for bounding the expected number of comparisons. Let $T(n)$ be the *expected* number of comparisons performed by Quicksort on an input of size n . In general, if the pivot is chosen to be the i^{th} order statistic of the input array,

$$T(n) = n - 1 + T(i - 1) + T(n - i).$$

where we define $T(0) = 0$. Each of the n possible choices of i are equally likely. Thus, the expected number of comparisons is:

$$\begin{aligned} T(n) &= n - 1 + \frac{1}{n} \sum_{i=1}^n \left(T(i - 1) + T(n - i) \right) \\ &= n - 1 + \frac{2}{n} \sum_{i=1}^{n-1} \left(T(i) \right) \end{aligned}$$

We use two facts:

1. $\sum_{i=1}^{n-1} f(i) \leq \int_1^n f(x) dx$ for an increasing function f
2. $\int 2x \ln x dx = x^2 \ln x - \frac{x^2}{2} + C$

Now we show that $T(n) \leq 2n \ln n$ by induction.

Base case: An array of size 1 is trivially sorted and requires no comparisons. Thus, $T(1) = 0$.

Inductive hypothesis: $T(i) \leq 2i \ln i$ for all $i < n$

Inductive step: We bound $T(n)$:

$$\begin{aligned} T(n) &= n - 1 + \frac{2}{n} \sum_{i=1}^{n-1} T(i) \\ &\leq n - 1 + \frac{2}{n} \sum_{i=1}^{n-1} 2i \ln i \\ &\leq n - 1 + \frac{2}{n} \int_1^n (2x \ln x) dx \\ &= n - 1 + \frac{2}{n} \left[n^2 \ln n - \frac{n^2}{2} + \frac{1}{2} \right] \\ &= 2n \ln n + n - 1 - n + \frac{1}{n} \\ &= 2n \ln n - 1 + \frac{1}{n} \\ &\leq 2n \ln n \end{aligned}$$

1 Hash tables

A hash table is a commonly used data structure to store an unordered set of items, allowing constant time inserts, lookups and deletes (in expectation). Every item consists of a unique identifier called a *key* and a piece of information. For example, the key might be a Social Security Number, a driver's license number, or an employee ID number. The way in which a hash table stores a item depends only on its key, so we will only focus on the key here, but keep in mind that each key is usually associated with additional information that is also stored in the hash table.

A hash table supports the following operations:

- $\text{INSERT}(k)$: Insert key k into the hash table.
- $\text{LOOKUP}(k)$: Check if key k is present in the table.
- $\text{DELETE}(k)$: Delete the key k from the table.

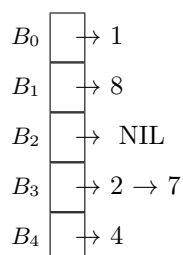
Each operation will take constant time (in expectation).

1.1 Implementation

Let U be the universe of all keys. For example, U could be the set of all 64 bit strings. In this case $|U| = 2^{64}$. This is a very large universe, but we do not need to store all of these 2^{64} keys, we only need to store a subset $S \subset U$. Suppose that we know that the size of the subset we will need to store is less than or equal to n , which is much less than the size of the universe $|U|$. In a hash table of size n , each key $k \in U$ is mapped to one of n "buckets" by a hash function $h : U \rightarrow \{1, 2, \dots, n\}$. Since the universe U is much larger than n , multiple keys could map to the same hash bucket. To accommodate this, each bucket contains a linked list of keys currently stored in that bucket.

Example

Suppose we have a hash table of size $n = 5$ with hash function $h(x) = 13x + 2 \pmod{5}$. After inserting the elements $\{1, 2, 4, 7, 8\}$ the hash table looks like this:



Where arrows denote pointers in the linked lists, and B_2 is empty. For example, 1 is placed into bucket B_0 because $h(1) = 15 \pmod{5} = 0$.

Time complexity

With this setup, the time required to perform an INSERT, LOOKUP or DELETE operation on key k is linear in the length of the linked list for the bucket that key k maps to. We just use the hash function to find the correct bucket for a input key k , and then search the corresponding linked list for the element, inserting or deleting if necessary. (Note that an INSERT could be performed in constant time by always inserting at the head of the list, but we first need to check if key k is already present).

Choice of size of hash table

The hash table size is usually chosen so that the size of the hash table is at least as large as the maximum number of keys we will need to store at any point of time. (If this condition is violated and the number of keys stored grows much larger than the size of the hash table, an implementation will usually increase the size of the table, and recompute the new table from scratch by mapping all keys to the bigger table. Our analysis ignores these complications and assumes that the number of keys is at most the hash table size.)

Potential problem with this implementation

In order for the operations to be implemented efficiently, we would like the keys to be distributed uniformly amongst the buckets in the hash table. We might hope that all buckets have at most a constant number of keys mapped to them, so that all operations could be performed in constant time. But for any fixed choice hash function h , one can always produce a subset of keys S such that all keys in S are mapped to the same location in the hash table. In this case, the running times of all operations will be linear in the number of keys – far from the constant we were hoping for. Thus, for a fixed hash function h , it is impossible to give worst case guarantees for the running times of hash table operations.

Possible solutions

There are two styles of analysis that we could use to circumvent this problem:

1. Assume that the set of keys stored in the hash table is random, or
2. Assume that the hash function h is random.

Both are plausible alternatives. The problem with the first alternative is that it is hard to justify that the set of keys stored in the hash table is truly random. It would be more satisfying to have an analysis that works for any subset of keys currently in the hash table. In these notes, we will explore the second alternative, i.e., assume that the hash function h is random.

1.2 Hashing with a completely random hash function

What does it mean for h to be random? One possibility is that h is chosen uniformly and at random from amongst the set of all hash functions $h : U \rightarrow \{1, 2, \dots, n\}$. In fact picking such a hash function is not really practical. Note that there are $n^{|U|}$ possible hash functions. Representing just one of these hash functions requires $\log(n^{|U|}) = |U| \log n$ bits. In fact, this means we need to write down $h(x)$ for every $x \in U$ in order to represent h . That's a lot of storage space! Much more than the size of the set we are trying to store in the hash table. One could optimize this somewhat by only recording $h(x)$ for all keys x seen so far (and generating $h(x)$ randomly on the fly when a new x is encountered), but this is impractical too. How would we check if a particular key x has already been encountered? Looks like we would need a hash table for that. But wait, isn't that what we set out to implement? Overall, it is clear that picking a completely random hash function is completely impractical.

Despite this, we will analyze hashing assuming that we have a completely random hash function and then explain how this assumption can be replaced by something that is practical.

Expected cost of hash table operations with random hash function

What is the expected cost of performing any of the operations INSERT, LOOKUP or DELETE with a random hash function? Suppose that the keys currently in the hash table are k_1, \dots, k_n . Consider an operation involving key k_i . The cost of the operation is linear in the size of the hash bucket that k_i maps to. Let X be the size of the hash bucket that k_i maps to. X is a random variable and

$$\begin{aligned} E[X] &= \sum_{j=1}^n \Pr[h(x_i) = h(x_j)] \\ &= 1 + \sum_{j \neq i} \Pr[h(x_i) = h(x_j)] \\ &= 1 + \frac{n-1}{n} \leq 2 \end{aligned}$$

Here the last step follows from the fact that $\Pr[h(x_i) = h(x_j)] = 1/n$ when h is random. Note that each key appears in the hash table at most once.

Thus the expected cost of any hashing operation is a constant.

1.3 Universal hash functions

Can we retain the expected cost guarantee of the previous section with a much simpler (i.e. practical) family of hash functions? In the analysis of the previous section, the only fact we used about random hash functions was that $\Pr[h(x_i) = h(x_j)] = 1/n$. Is it possible to construct a small, practical subset of hash functions with this property?

Thinking along these lines, in 1978, Carter and Wegman introduced the notion of *universal hashing*: Consider a family F of hash functions from U to $\{1, 2, \dots, n\}$. We say that F is universal if, for every $x_i \neq x_j$, for a h chosen randomly from F , $\Pr[h(x_i) = h(x_j)] \leq 1/n$.

Clearly the analysis of the previous section shows that for any universal family, the constant expected running time guarantee applies. The family of all hash functions is universal. Is there a simpler universal family?

1.4 A universal family of hash functions

Suppose that the elements of the U are encoded as non-negative integers in the range $\{0, \dots, |U| - 1\}$. Pick a prime $p \geq |U|$. For $a, b \in \{0, \dots, p-1\}$, consider the family of hash functions

$$h_{a,b}(x) = ax + b \mod p \mod n$$

where $a \in [1, p-1]$ and $b \in [0, p-1]$.

Proposition 1. *This family of hash functions F is universal.*

In order to prove this statement, first, let's count the number of hash functions in this family F . We have $p-1$ choices for a , and p choices for b , so $|F| = p(p-1)$. In order to prove that F is universal, we need to show that for a h chosen randomly from F , $\Pr[h(x_i) = h(x_j)] \leq 1/n$. Since there are $p(p-1)$ hash functions in F , this is equivalent to showing that the number of hash functions in F that map x_i and x_j to the same output is less than or equal to $\frac{p(p-1)}{n}$. To show that this is true, first consider how $h_{a,b}$ behaves without the mod n . Call these functions $f_{a,b}$:

$$f_{a,b}(x) = ax + b \mod p$$

The $f_{a,b}$ have the following useful property:

Claim 1. For a given $x_1, x_2, y_1, y_2 \in [0, p-1]$ such that $x_1 \neq x_2$ there exists only one function $f_{a,b}$ such that

$$\begin{aligned} f_{a,b}(x_1) &= y_1 \text{ AND} \\ f_{a,b}(x_2) &= y_2 \end{aligned}$$

Proof. Solve the above two equations for a and b :

$$\begin{aligned} ax_1 + b &\equiv y_1 \pmod{p} \\ ax_2 + b &\equiv y_2 \pmod{p} \end{aligned}$$

By subtracting the two equations, we get:

$$a(x_1 - x_2) \equiv y_1 - y_2 \pmod{p}$$

Since p is prime and $x_1 \neq x_2$, the above equation has only one solution for $a \in [0, p-1]$. Then

$$b \equiv y_1 - ax_1 \pmod{p}$$

So we have found the unique a and b such that $f_{a,b}(x_1) = y_1$ and $f_{a,b}(x_2) = y_2$. \square

In the above proof, note that $a = 0$ only when $y_1 = y_2 = b$. This is why we restrict $a \neq 0$, we don't want the hash function mapping all elements to the same value b .

Now, we have shown that for a given x_1, x_2 , for each selection of y_1, y_2 with $y_1 \neq y_2$, there is exactly one function $f_{a,b}$ that maps x_1 to y_1 and x_2 to y_2 . So, in order to find out how many functions $h_{a,b}$ map x_1 and x_2 to the same value mod n , we just need to count the number of pairs (y_1, y_2) where $y_1 \neq y_2$ and $y_1 \equiv y_2 \pmod{n}$. There are p possible selections of y_1 for this pair, and then $\leq (p-1)/n$ of the possibilities for y_2 will be equal to $y_1 \pmod{n}$. (Convince yourself that this is true.) This gives a total of $\frac{p(p-1)}{n}$ functions $h_{a,b}$ that map x_1 and x_2 to the same element. So then

$$\begin{aligned} Pr[h_{a,b}(x_1) = h_{a,b}(x_2)] &\leq \frac{p(p-1)/n}{|F|} \\ &= \frac{p(p-1)}{p(p-1)(n)} \\ &= \frac{1}{n} \end{aligned}$$

which means the family F of the $h_{a,b}$ is universal, as desired. \square

Wrapping up the discussion on hashing, if we pick a random hash function from this family, then the expected cost of any hashing operation is constant. Note that picking a random hash function from the family simply involves picking a, b – significantly simpler than picking a completely random hash function.

2 Balls and Bins

A useful abstraction in thinking about hashing with random hash functions is the following experiment: Throw m balls randomly into n bins. (The connection to hashing should be clear: the balls represent the keys and the bins represent the hash buckets.) The balls into bins experiment arises in several other problems as well, e.g., analysis of load balancing. In the context of hashing, the following questions arise about the balls and bins experiment:

- How large does m have to be so that with probability greater than $1/2$, we have (at least) two balls in the same bin? This tells us how large our hash table needs to be to avoid any collisions. We will explore this at the end of these notes.
- Suppose $m = n$; what is the maximum number of balls that fall into a bin? This tells us the size of the largest bucket in the hash table when the number of keys is equal to the number of buckets in the table. We might explore this in the next homework.

No collisions

The first question is related to the so called *birthday paradox*: Suppose you have 23 people in a room. Then (somewhat surprisingly) the probability that there exists some pair with the same birthday is greater than $1/2$! (This assumes that birthdays are independent and randomly distributed.) 23 seems like an awfully small number to get a pair with the same birthday. There are 365 days in a year! How do we explain this? Consider throwing m balls into n bins. The expected number of pairs that fall into the same bucket is $m(m-1)/2n$. (This follows from linearity of expectation. Note that the probability that a fixed pair falls into the same bucket is $1/n$.) Thus the probability that there is a collision is upper bounded by the expected number of collisions which is $m(m-1)/2n$. (Convince yourself that this is true.) On the other hand, we can also show that the probability that all m balls fall into distinct bins is at most $e^{-m(m-1)/2n}$.

Proof.

$$P[\text{no collisions}] = \prod_{i=1}^{m-1} \left(1 - \frac{i}{n}\right)$$

Now, we use the fact that $(1-x) \leq e^{-x}$:

$$\left(1 - \frac{i}{n}\right) \leq e^{-i/n}$$

So

$$P[\text{no collisions}] \leq \prod_{i=1}^{m-1} e^{-i/n}$$

$$P[\text{no collisions}] \leq e^{\sum_{i=1}^{m-1} -i/n}$$

$$P[\text{no collisions}] \leq e^{(-m(m-1)/(2n))}$$

□

For m about $\sqrt{(2 \ln 2)n} \approx 1.18\sqrt{n}$ this probability is less than $1/2$, i.e. the probability of a collision is greater than $1/2$.

This is a useful design principle to keep in mind: If we want to design a hash table with no collisions, then the size of the hash table should be larger than the square of the number of elements we need to store in it. For our purposes in this note, insisting on no collisions means that the number of elements in the hash table can only be a small fraction of the hash table size which is quite wasteful.

The birthday problem calculation is useful in other contexts. Here is an application: Suppose we assign random b -bit IDs to m users. How large does b have to be to ensure that all users have distinct IDs with probability $1 - \delta$. Here $\delta > 0$ is a given error tolerance. Assigning b -bit IDs is identical to mapping to $n = 2^b$ buckets. The birthday problem calculation shows us that the probability of a collision is at most $m^2/2n = m^2/2^{b+1}$. We should set b large enough such that this bound is at most δ . Thus b should be at least $2 \log m - 1 + \log(1/\delta)$.

1 Data Structures

Thus far in this course we have mainly discussed algorithm design, and have specified algorithms at a relatively high level. For example, in describing sorting algorithms, we often assumed that we could insert numbers into a list in constant time; we didn't worry too much about the actual implementation of this, and took it as an assumption that this could actually be implemented (e.g. via a linked-list).

In this lecture, we will talk about the actual design and implementation of some useful data-structures. The purpose of this lecture is mainly to give you a taste of data-structure design. We won't discuss this area too much more in the course, and will switch back to discussing higher-level algorithms. If you like data-structures, CS166 is an entire course about them!

To motivate the data structures that we will discuss in this lecture, consider the following table that lists a bunch of basic operations that we would like to perform on a set/list of numbers, together with the worst-case runtime of performing those operation for two of the data structures that you are (hopefully) familiar with: linked lists of n sorted numbers, and an array of n sorted numbers:

Operation	Runtime with Sorted Linked List	Runtime with Sorted Array
Search (i.e. find 17)	$\Theta(n)$	$\Theta(\log n)$ (via binary search)
Select (i.e. find 12 smallest element)	$\Theta(n)$	$\Theta(1)$ (just look at 12th elt.)
Rank (i.e. # elt. less than 17)	$\Theta(n)$	$\Theta(\log n)$
Predecessor/Sucessor ¹	$\Theta(1)$	$\Theta(1)$
Insert element	$\Theta(1)$	$\Theta(n)$
Delete element	$\Theta(1)$	$\Theta(n)$

In the above table, the time to insert or delete an element in a linked list is $\Theta(1)$ provided we are specifying where to insert/delete the element via pointers. (If we specify the *value* to insert/delete, then the time is $\Theta(n)$, since we first need to search for that element....)

The above table makes Sorted Arrays look like a pretty decent datastructure for *static* data. In many applications, however, the data changes often, in which case the $\Theta(n)$ time it takes to insert or delete an element is prohibitive. This prompts the question: *Is it possible to have one data structure that is the best of both worlds (logarithmic or constant time for all these operations)?* The answer is, essentially, "Yes", provided we don't mind if some of the $\Theta(1)$'s turn into $\Theta(\log n)$. We now sketch out one such datastructure, the *Binary Search Tree*.

2 Binary Search Trees

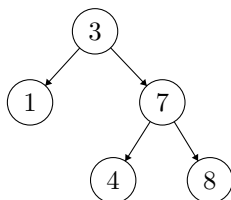
Definition 2.1. A binary search tree (BST) is a data structure that stores elements that have keys from a totally ordered universe (say, the integers). In this lecture, we will assume that each element has a unique key. A BST supports the following operations:

- $\text{search}(i)$: Returns an element in the data structure associated with key i
- $\text{insert}(i)$: Inserts an element with key i into the data structure
- $\text{delete}(i)$: Deletes an element with key i from the data structure, if such an element exists

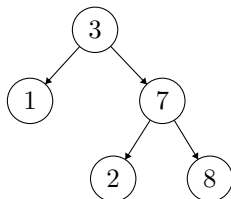
A BST stores the elements in a binary tree with a root r . Each node x has $\text{key}(x)$ (the key of the element stored in x), $p(x)$ (the parent of x , where $p(r) = \text{NIL}$), $\text{left}(x)$ (the left child of x), and $\text{right}(x)$ (the right child of x). The children of x are either other nodes or NIL .

The key BST property is that for every node x , the keys of all nodes under $\text{left}(x)$ are less than $\text{key}(x)$ and the keys of all nodes under $\text{right}(x)$ are greater than $\text{key}(x)$.

Example In the following example, the root node r stores 3 in it ($\text{key}(r) = 3$), its left child $\text{left}(x)$ stores 1, its right child $\text{right}(x)$ stores 7, and all leaf nodes (storing 1, 4, and 8, respectively) have NIL as their two children.



Example The following binary tree is not a BST since $2 > 3$ and 2 is a child of 7, which is the right child of 3:



Some properties. *Relationship to Quicksort:* We can think of each node x as a pivot for quicksort for the keys in its subtree. The left subtree contains $A_{<}$ for $\text{key}(x)$ and the right subtree contains $A_{>}$ for $\text{key}(x)$.

Sorting the keys: We can do an *inorder* traversal of the tree to recover the nodes in sorted order from left to right (the smallest element is in the leftmost node and the largest element is in the rightmost node). The *lnorder* procedure takes a node x and returns the keys in the subtree under x in sorted order. We can recursively define *lnorder*(x) as: (1) If $\text{left}(x) \neq \text{NIL}$, then run *lnorder*($\text{left}(x)$), then: (2) Output $\text{key}(x)$ and then: (3) If $\text{right}(x) \neq \text{NIL}$, run *lnorder*($\text{right}(x)$). With this approach, for every x , all keys in its left subtree will be output before x , then x will be output and then every element in its right subtree.

Subtree property: If we have a subtree where x has y as a left child, y has z as a right child, and z is the root for the subtree T_z , then our BST property implies that all keys in T_z are $> y$ and $< x$. Similarly, if we have a subtree where x has y as a right child, y has z as a left child, and z is the root of the subtree T_z , then our BST property implies that all keys in T_z are between x and y .

2.1 Basic Operations on BSTs

The three core operations on a BST are **search**, **insert**, and **delete**. For this lecture, we will assume that the BST stores distinct numbers, i.e. we will identify the objects with their names and we will have each name be represented by a number.

2.1.1 search

To **search** for an element, we start at the root and compare the key of the node we are looking at to the element we are searching for. If the node's key matches, then we are done. If not, we recursively search in the left or right subtree of our node depending on whether this node was too large or too small, respectively. If we ever reach NIL , we know the element does not exist in our BST. In the following algorithm in this case, we simply return the node that would be the parent of this node if we inserted it into our tree.

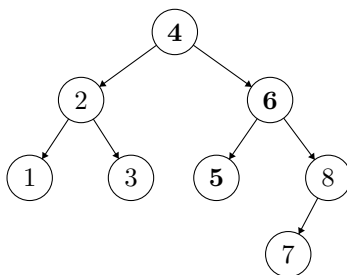
Algorithm 1: $\text{search}(i)$

return $\text{search}(\text{root}, i);$

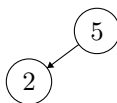
Algorithm 2: $\text{search}(x, i)$

```
if  $\text{key}(x) == i$  then
  return  $x$ 
else if  $i < \text{key}(x)$  then
  if  $\text{left}(x) == \text{NIL}$  then
    return  $x$ 
  else
    return  $\text{search}(\text{left}(x), i)$ 
else if  $i > \text{key}(x)$  then
  if  $\text{right}(x) == \text{NIL}$  then
    return  $x$ 
  else
    return  $\text{search}(\text{right}(x), i)$ 
```

Example If we call $\text{search}(5.5)$ on the following BST, we will return the node storing 5 (by taking the path in bold). This also corresponds to the path taken when calling $\text{search}(4.5)$ or $\text{search}(5)$.



Claim 1. $\text{search}(i)$ returns a node containing i if $i \in \text{BST}$, otherwise a node x such that either $\text{key}(x)$ is the smallest in $\text{BST} > i$ or the largest in $\text{BST} < i$, where node x happens to be the parent of the new node if it were to be inserted into BST . This follows directly from the BST property. Try to formally prove this claim as an exercise.



Remark 1. $\text{search}(i)$ does **not** necessarily return the node in BST that is closest in value. Consider the tree above. If we search for an element with a key of 4, the node with key 2 is returned, whereas the element with key 5 is the closest element by value.

2.1.2 insert

As before, we will assume that all keys are distinct. We will $\text{search}(i)$ for a node x to be the parent and create a new node y , placing it as a child of x where it would logically go according to the BST property.

Remark 2. Notice that x needed to have NIL as a child where we want to put y by the properties of our search algorithm.

Algorithm 3: insert(i)

```
 $x \leftarrow \text{search}(i);$   
 $y \leftarrow$  new node with  $\text{key}(y) \leftarrow i$ ,  $\text{left}(y) \leftarrow \text{NIL}$ ,  $\text{right}(y) \leftarrow \text{NIL}$ ,  $\text{p}(y) \leftarrow x$ ;  
if  $i < \text{key}(x)$  then  
|    $\text{left}(x) \leftarrow y$ ;  
else  
|    $\text{right}(x) \leftarrow y$ ;
```

2.1.3 delete

Deletion is a bit more complicated. To delete a node x that exists in our tree, we consider several cases:

1. If x has no children, we simply remove it by modifying its parent to replace x with NIL.
2. If x has only one child c , either left or right, then we elevate c to take x 's position in the tree by modifying the appropriate pointer of x 's parent to replace x with c , and also fixing c 's parent pointer to be x 's parent.
3. If x has two children, a left child c_1 and right child c_2 , then we find x 's immediate successor z and have z take x 's position in the tree. Notice that z is in the subtree under x 's right child c_2 and we can find it by running $z \leftarrow \text{search}(c_2, \text{key}(x))$. Note that since z is x 's successor, it doesn't have a left child, but it might have a right child. If z has a right child, then we make z 's parent point to that child instead of z (also fixing the child's parent pointer). Then we replace x with z , fixing up all relevant pointers: the rest of x 's original right subtree becomes z 's new right subtree, and x 's left subtree becomes z 's new left subtree.

(Note that alternatively, we could have used x 's immediate predecessor y and followed the same analysis in a mirrored fashion.)

In the following algorithm, if p is the parent of x , $\text{child}(p)$ refers to $\text{left}(p)$ if x was the left child of p and to $\text{right}(p)$ otherwise.

2.1.4 Runtimes

The worst-case runtime for `search` is $O(\text{height of tree})$. As both `insert` and `delete` call `search` a constant number of times (once or twice) and otherwise perform $O(1)$ work on top of that, their runtimes are also $O(\text{height of tree})$.

In the best case, the height of the tree is $O(\log n)$, e.g., when the tree is completely balanced. However, in the worst case it can be $O(n)$ (a long rightward path, for example). This could happen because `insert` can increase the height of the tree by 1 every time it is called. Currently our operations do not guarantee logarithmic runtimes. To get $O(\log n)$ height we would need to rebalance our tree. There are many examples of self-balancing BSTs, including AVL trees, red-black trees, splay trees (somewhat different but super cool!), etc. Today, we will talk about red-black trees.

3 Red-Black Trees

One of the most popular balanced BST is the red-black tree developed by Guibas and Sedgwick in 1978. In a red-black tree, all leaves are assumed to have NILs as children.

Definition 3.1. A red-black tree is a BST with the following additional properties:

1. Every node is red or black
2. The root is black

Algorithm 4: delete(i)

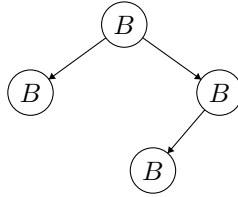
```
 $x \leftarrow \text{search}(i);$ 
if  $\text{key}(x) \neq i$  then return;
if  $\text{NIL} = \text{left}(x)$  and  $\text{NIL} = \text{right}(x)$  then
     $\text{child}(\text{p}(x)) \leftarrow \text{NIL};$ 
     $\text{delete-node}(x);$ 
if  $\text{NIL} = \text{left}(x)$  then
     $y \leftarrow \text{right}(x);$ 
     $\text{p}(y) \leftarrow \text{p}(x);$ 
     $\text{child}(\text{p}(y)) \leftarrow y;$ 
     $\text{delete-node}(x);$ 
else if  $\text{NIL} = \text{right}(x)$  then
     $y \leftarrow \text{left}(x);$ 
     $\text{p}(y) \leftarrow \text{p}(x);$ 
     $\text{child}(\text{p}(y)) \leftarrow y;$ 
     $\text{delete-node}(x);$ 
else  $x$  has two children
     $z \leftarrow \text{search}(\text{right}(x), \text{key}(x));$ 
     $z' \leftarrow \text{right}(z);$ 
     $\text{left}(\text{p}(z)) \leftarrow z';$ 
     $\text{p}(z') \leftarrow \text{p}(z);$ 
    replace  $x$  with  $z;$ 
     $\text{delete-node}(x);$ 
```

3. NILs are black

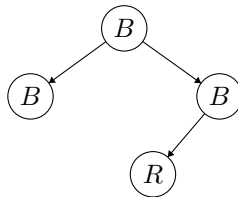
4. The children of a red node are black

5. For every node x , all x to NIL paths have the same number of black nodes on them

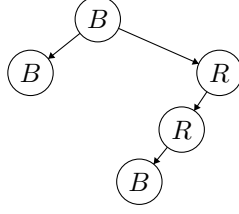
Example (B means a node is black, R means a node is red.) The following tree is *not* a red-black tree since since property 5 is not satisfied:



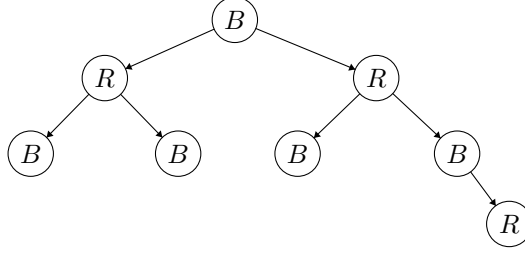
Example (B means a node is black, R means a node is red.) The following tree *is* a red-black tree since all the properties are satisfied:



Example (B means a node is black, R means a node is red.) The following tree is *not* a red-black tree since property 4 is not satisfied:



Example (B means a node is black, R means a node is red.) The following tree *is* a red-black tree:



Remark 3. Intuitively, red nodes represent when a path is becoming too long.

Claim 2. Any valid red-black tree on n nodes (non-NIL) has height $\leq 2\log_2(n+1) = O(\log n)$.

Proof. For some node x , let $b(x)$ be the “black height” of x , which is the number of black nodes on a $x \rightarrow \text{NIL}$ path excluding x . We first show that the number of non-NIL descendants of x is at least $2^{b(x)} - 1$ (including x) via induction on the height of x .

Base case: NIL node has $b(x) = 0$ and $2^0 - 1 = 0$ non-NIL descendants. ✓

For our inductive step, let $d(x)$ be the number of non-NIL descendants of x . Then

$$\begin{aligned} d(x) &= 1 + d(\text{left}(x)) + d(\text{right}(x)) \\ &\geq 1 + (2^{b(x)-1} - 1) + (2^{b(x)-1} - 1) \text{ (by induction)} \\ &= 2^{b(x)} - 1 \text{ ✓} \end{aligned}$$

Notice that $b(x) \geq \frac{h(x)}{2}$ (where $h(x)$ is the height of x) since on any root to NIL path there are no two consecutive red nodes, so the number of black nodes is at least the number of red nodes, and hence the black height is at least half of the height. We apply this and the above inequality to the root r (letting $h = h(r)$) to obtain $n \geq 2^{b(r)} - 1 \geq 2^{\frac{h}{2}} - 1$, and hence $h \leq 2\log(n+1)$. □

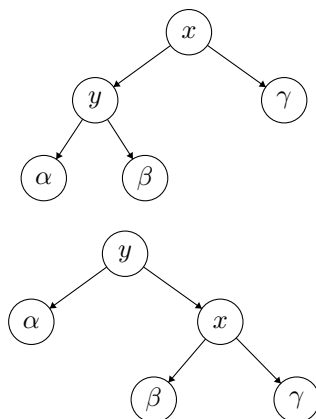
Here is some intuition on why the tree is roughly balanced.

Intuition: By Property (5) of a red-black tree, all $r \rightarrow \text{NIL}$ paths have $b(r)$ black nodes (excluding the root). Therefore, all these paths have length $\geq b(r)$. However, they also have length $\leq 2 \cdot b(r)$: by Property (4), the number of red nodes is limited to half of the path, since every red node must be followed by a black node, and hence the number of black nodes is at least half of the length of the path. Hence, the lengths of all paths from r to a NIL are within a factor of 2 of each other, and the tree must be reasonably balanced.

Today we will take a brief look at how the red-black tree properties are maintained. Our coverage here is detailed, but not comprehensive, and meant as a case study. For complete coverage, please refer to Ch. 13 of CLRS.

3.1 Rotations

Red-black trees, as do other balanced BSTs, use a concept called rotation. A tree rotation restructures the tree shape locally, usually for the purpose of balancing the tree better. A rotation preserves the BST property (as shown in the following two diagrams). Notably, tree rotations can be performed in $O(1)$ time.



Moving from the first tree to the second is known as a *right rotation of x* . The other direction (from the second tree to the first) is a *left rotation of y* . Notice that we only move the β subtree, which is why we preserve the BST property.

3.2 Insertion in a Red-Black Tree

Let's see how we can perform $\text{Insert}(i)$ on a red-black tree while still maintaining all of its properties. The process for inserting a new node is initially similar to that of insertion into any BST.

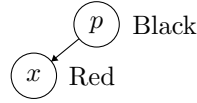
Algorithm 5: insert_rb(i)

```
 $p \leftarrow \text{search}(i);$   
 $x \leftarrow$  new node with  $\text{key}(x) \leftarrow i$ ,  $\text{left}(x) \leftarrow \text{NIL}$ ,  $\text{right}(x) \leftarrow \text{NIL}$ ,  $\text{p}(x) \leftarrow p$ ;  
if  $i < \text{key}(p)$  then  
|  $\text{left}(p) \leftarrow x$ ;  
else  
|  $\text{right}(p) \leftarrow x$ ;  
 $\text{color}(x) \leftarrow \text{red}$ ;  
recolor if needed;
```

Note that when x is inserted as a red node: Property (1) is satisfied, as we colored the new node red; Property (2) is satisfied, as we did not touch the root; Property (3) is satisfied, as we can color the new NILs black; and Property (5) is satisfied, as we did not change the number of black nodes in the tree. Thus, the only invariant we have to worry about is Property (4), that red nodes have black children.

The recoloring step is broken down into multiple cases. We consider each of them:

Case 1: p is black. In this case, Property (4) is also maintained. So, we simply add x as a new red child of p , and the red-black tree properties are maintained.



Case 2: p is red, and x 's uncle u is red. In this case, we insert a red x , change p and u to black, and change p' to red. Because we switched the colors of two nodes on each of these paths (one red→black and one black→red), the number of black nodes on each path is unchanged, so Property (5) remains unchanged. If the parent of p' , p'' , is black, then Property (4) is maintained. Otherwise, if p'' is red and breaks Property (4) by introducing a “double-red” pair of nodes (p' and p''), then we have to recolor recursively starting at p' .



Case 3: p is red, and u is black. There are two possibilities here:

1. We are inserting x as a leaf node. Then, u must be NIL for the red-black tree to have been valid before inserting x . We insert a red x .
2. We are not inserting x ; rather, we are recoloring the tree at x from the recursive call in Case 2. We aim to recolor the tree and maintain the number of black nodes on each path from the root to NIL. Note that in this case, x actually has nodes under it.

In both cases, x is red, so we make p black, make p' red, and do a right rotation at p' . We can see that this also maintains the same number of black nodes on each path from the root to NIL, and satisfies Property (4) below p because the original tree was a red-black tree.



If we end up in Case 2 and recursively call `recolor`, then in the worst case the recursion will bottom out when we hit the root, with a constant number of relabelings and rotations at each level. So, it will be an $O(h)$ operation overall, where h is the height of the tree.

In the analysis above, we considered the cases where x is a left child of p and u is a right child of its parent p' . These cases are representative, showing most of the machinery that we'll need to insert an arbitrary element into an arbitrary red-black tree. (Within Case 2 and Case 3, there are actually a total of four cases each, where p 's tree and p' 's children could each be swapped, but the recoloring procedure is similar. You are encouraged to read the text for details.)

To summarize, the following is the algorithm for recoloring, in the case where x is a left child and u is a right child.

Algorithm 6: `recolor(x)` // x is a left child, u is a right child

```

 $p \leftarrow \text{parent}(x);$ 
if  $\text{black} = \text{color}(p)$  then
     $\text{return};$ 
 $p' \leftarrow \text{parent}(p);$ 
 $u \leftarrow \text{right}(p');$ 
if  $\text{red} = \text{color}(u)$  then
     $\text{color}(p) \leftarrow \text{black};$ 
     $\text{color}(u) \leftarrow \text{black};$ 
     $\text{color}(p') \leftarrow \text{red};$ 
     $\text{recolor}(p');$ 
else if  $\text{black} = \text{color}(u)$  then
     $\text{color}(p) \leftarrow \text{black};$ 
     $\text{color}(p') \leftarrow \text{red};$ 
     $\text{right\_rotate}(p');$ 

```

Based on our analysis above, we can update our red-black trees in $O(h)$ time upon insertion, where h is the height of the tree. The other operations are similar, and also give the guarantee of worst-case performance of $O(h)$ search, insertion, and deletion. Together with Claim 2, which states that $h = O(\log n)$, we get:

Claim 3. *Red-black trees support insert, delete, and search in $O(\log n)$ time.*

As we have seen, BSTs are very nice – they allow us to maintain a set and report membership, insert, and delete in $O(\log n)$ time. In addition to these basic underlying operations, we can also support other types of queries efficiently. Because the elements are stored maintaining the binary search tree property, we can search for the next largest element or the elements on a range very efficiently. But what if we don't care about these properties? What if we only need to support membership queries? Can we improve our performance of $O(\log n)$ time to nearly constant time? This question motivates our discussion of hash tables, which we will cover in the next lecture.

1 Graphs

A **graph** is a set of **vertices** and **edges** connecting those vertices. Formally, we define a graph G as $G = (V, E)$ where $E \subseteq V \times V$. For ease of analysis, the variables n and m typically stand for the number of vertices and edges, respectively. Graphs can come in two flavors, **directed** or **undirected**. If a graph is undirected, it must satisfy the property that $(i, j) \in E$ iff $(j, i) \in E$ (i.e., all edges are bidirectional). In undirected graphs, $m \leq \frac{n(n-1)}{2}$. In directed graphs, $m \leq n(n-1)$. Thus, $m = O(n^2)$ and $\log m = O(\log n)$. A connected graph is a graph in which for any two nodes u and v there exists a path from u to v . For an undirected connected graph $m \geq n - 1$. A *sparse graph* is a graph with few edges (for example, $\Theta(n)$ edges) while a *dense graph* is a graph with many edges (for example, $m = \Theta(n^2)$).

1.1 Representation

A common issue is the topic of how to represent a graph's edges in memory. There are two standard methods for this task.

An **adjacency matrix** uses an arbitrary ordering of the vertices from 1 to $|V|$. The matrix consists of an $n \times n$ binary matrix such that the $(i, j)^{th}$ element is 1 if (i, j) is an edge in the graph, 0 otherwise.

An **adjacency list** consists of an array A of $|V|$ lists, such that $A[u]$ contains a linked list of vertices v such that $(u, v) \in E$ (the neighbors of u). In the case of a directed graph, it's also helpful to distinguish between outgoing and ingoing edges by storing two different lists at $A[u]$: a list of v such that $(u, v) \in E$ (the out-neighbors of u) as well as a list of v such that $(v, u) \in E$ (the in-neighbors of u).

What are the tradeoffs between these two methods? To help our analysis, let $\deg(v)$ denote the **degree** of v , or the number of vertices connected to v . In a directed graph, we can distinguish between out-degree and in-degree, which respectively count the number of outgoing and incoming edges.

- The adjacency matrix can check if (i, j) is an edge in G in constant time, whereas the adjacency list representation must iterate through up to $\deg(i)$ list entries.
- The adjacency matrix takes $\Theta(n^2)$ space, whereas the adjacency list takes $\Theta(m + n)$ space.
- The adjacency matrix takes $\Theta(n)$ operations to enumerate the neighbors of a vertex v since it must iterate across an entire row of the matrix. The adjacency list takes $\deg(v)$ time.

What's a good rule of thumb for picking the implementation? One useful property is the sparsity of the graph's edges. If the graph is **sparse**, and the number of edges is considerably less than the max ($m \ll n^2$), then the adjacency list is a good idea. If the graph is **dense** and the number of edges is nearly n^2 , then the matrix representation makes sense because it speeds up lookups without too much space overhead. Of course, some applications will have lots of space to spare, making the matrix feasible no matter the structure of the graphs. Other applications may prefer adjacency lists even for dense graphs. Choosing the appropriate structure is a balancing act of requirements and priorities.

2 Depth First Search (DFS)

Given a starting vertex, it's desirable to find all vertices reachable from the start. There are many algorithms to do this, the simplest of which is depth-first search. As the name implies, DFS enumerates the deepest

paths, only backtracking when it hits a dead end or an already-explored section of the graph. DFS by itself is fairly simple, so we introduce some augmentations to the basic algorithm.

- To prevent loops, DFS keeps track of a “color” attribute for each vertex. Unvisited vertices are white by default. Vertices that have been visited but still may be backtracked to are colored gray. Vertices which are completely processed are colored black. The algorithm can then prevent loops by skipping non-white vertices.¹
- Instead of just marking visited vertices, the algorithm also keeps track of the tree generated by the depth-first traversal. It does so by marking the “parent” of each visited vertex, aka the vertex that DFS visited immediately prior to visiting the child.
- The augmented DFS also marks two auto-incrementing timestamps d and f to indicate when a node was first discovered and finished.

The algorithm takes as input a start vertex s and a starting timestamp t , and returns the timestamp at which the algorithm finishes. Let $N(s)$ denote the neighbors of s ; for a directed graph, let $N_{out}(s)$ denote the out-neighbors of s .

Algorithm 1: $\text{init}(G)$

```

foreach  $v \in G$  do
     $\text{color}(v) \leftarrow \text{white}$ 
     $d(v), f(v) \leftarrow \infty$ 
     $p(v) \leftarrow \text{nil}$ 

```

Algorithm 2: $\text{DFS}(s, t)$ $s \in V$. $t = \text{time}$, s is white

```

 $\text{color}(s) \leftarrow \text{gray}$ 
 $\backslash\backslash$   $d(s)$  is the discovery time of  $s$ 
 $d(s) \leftarrow t$ 
 $t++$ ;
 $\backslash\backslash$  In the loop below, replace  $N(s)$  with  $N_{out}(s)$  for directed  $G$ 
foreach  $v \in N(s)$  do
    if  $\text{color}(v) = \text{white}$  then
         $p(v) \leftarrow s$ 
         $\backslash\backslash$  update  $t$  to be the finish time of DFS starting at  $v$ :
         $t \leftarrow \text{DFS}(v, t)$ 
         $t++$ 
 $\backslash\backslash$  finish time
 $f(s) \leftarrow t$ 
 $\backslash\backslash$   $s$  is finished
 $\text{color}(s) \leftarrow \text{black}$ 
return  $f(s)$ 

```

There are multiple ways we can search using DFS. One way is to search from some source node s , which will give us a set of black nodes reachable from s and white nodes unreachable from s .

Algorithm 3: $\text{DFS}(s)$ $\backslash\backslash$ DFS from a source node s

```

 $\text{init}(G)$ 
 $\text{DFS}(S, 1)$ 

```

Another way to use DFS is to search over the entire graph, choosing some white node and finding everything we can reach from that node, and repeating until we have no white nodes remaining. In an undirected graph this will give us all of the connected components.

¹In the slides, white, gray, and black are replaced with light green, orange, and dark green, respectively.

Algorithm 4: DFS(G) \\\ DFS on an entire graph G

```
init( $G$ );  
 $t \leftarrow 1$   
foreach  $v \in G$  do  
    if  $color(v) = white$  then  
         $t \leftarrow \text{DFS}(v, t)$   
         $t++$ 
```

2.1 Runtime of DFS

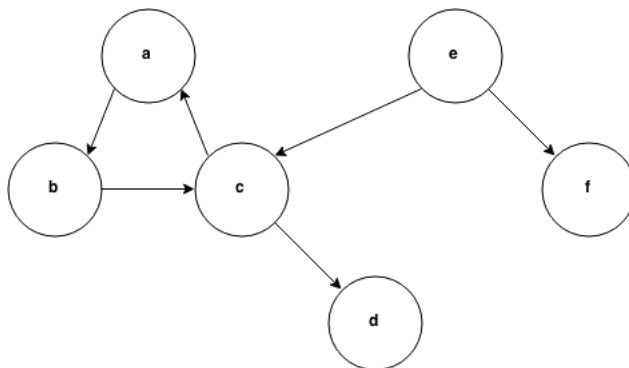
We will now look at the runtime for the standard DFS algorithm (Algorithm 2).

Everything above the loop runs in $O(1)$ time per node visit. Excluding the recursive call, everything inside of the for loop takes $O(1)$ time every time an edge is scanned. Everything after the for loop also runs in $O(1)$ time per node visit.

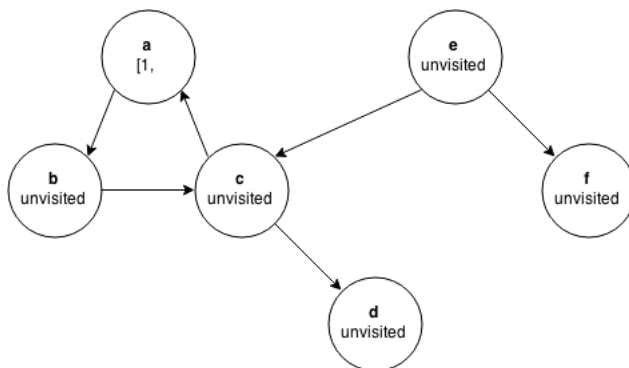
We can express the runtime of DFS as $O(\# \text{ of node visits} + \# \text{ of edge scans})$. Assume we have a graph with n nodes and m edges. We know that the $\#$ of node visits is $\leq n$, since we only visit white nodes and whenever we visit a node we change its color from white to gray and never change it back to white again. We also know that an edge (u, v) is scanned only when u or v is visited. Since every node is visited at most once, we know that an edge (u, v) is scanned at most twice (or only once for directed graphs). Thus, $\#$ of edges scanned is $O(m)$, and the overall runtime of DFS is $O(m + n)$.

2.2 DFS Example

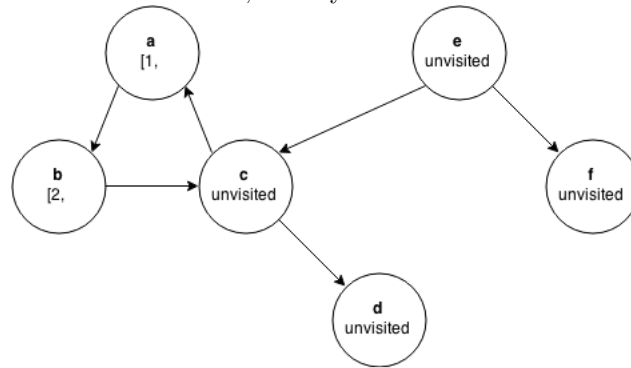
We will now try running DFS on the example graph below.



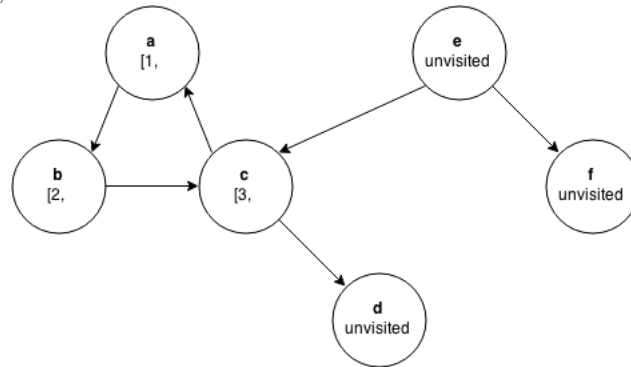
We mark all of the nodes as unvisited and start at a white node, in our case node a.



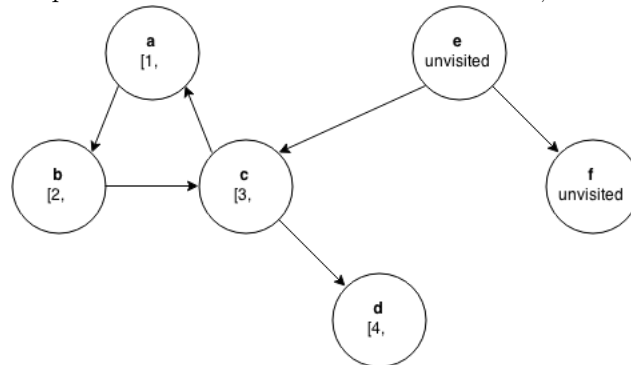
From node a we will visit all of a's children, namely node b.



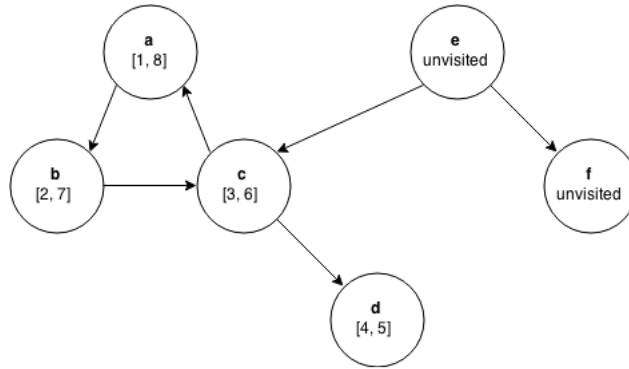
We now visit b's child, node c.



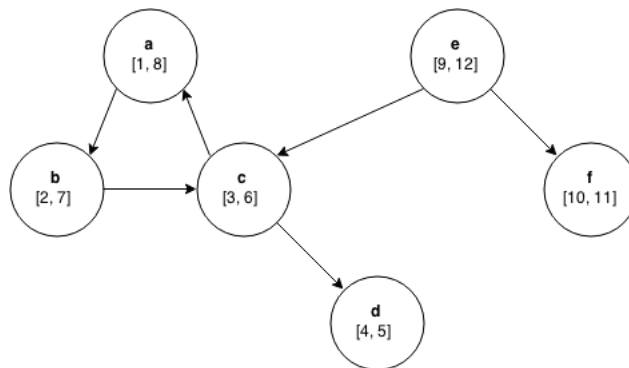
Node c has two children that we must visit. When we try to visit node a we find that node a has already been visited (and would be colored gray, as we are in the process of searching a's children), so we do not continue searching down that path. We will next search c's second child, node d.



Since node d has no children, we return back to its parent node, c, and continue to go back up the path we took, marking nodes with a finish time when we have searched all of their children.



Once we reach our first source node a we find that we have searched all of its children, so we look in the graph to see if there are any unvisited nodes remaining. For our example, we start with a new source node e and run DFS to completion.

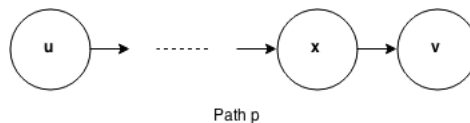


3 Breadth First Search (BFS)

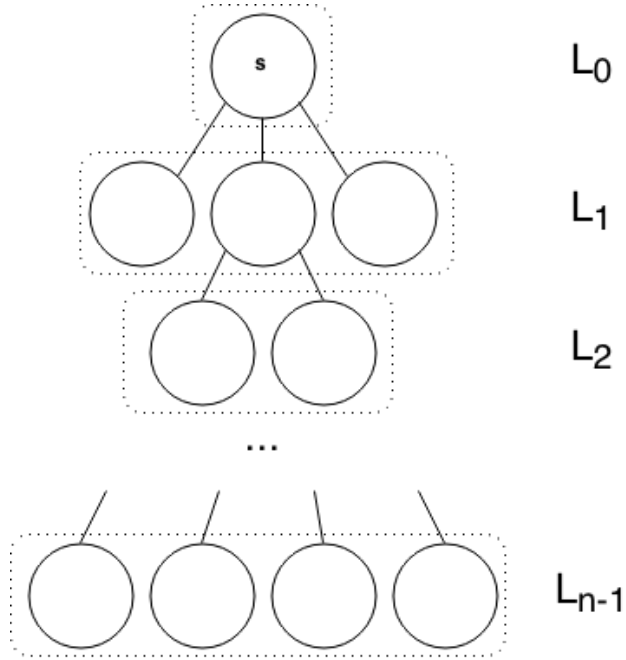
In depth first search, we search “deeper” in the graph whenever possible, exploring edges out of the most recently discovered node that still has unexplored edges leaving it. Breadth first search (BFS) instead expands the frontier between discovered and undiscovered nodes uniformly across the breadth of the frontier, discovering all nodes at a distance k from the source node before nodes at distance $k + 1$.

$\text{BFS}(s)$ computes for every node $v \in G$ the distance from s to v in G . $d(u, v)$ is the length of the shortest path from u to v .

A simple property of unweighted graphs is as follows: let P be a shortest $u \rightarrow v$ path and let x be the node before v on P . Then $d(u, v) = d(u, x) + 1$.



$\text{BFS}(s)$ computes sets L_i , the set of nodes at distance i from s , as seen in the diagram below.



Algorithm 5: BFS(s)

```

Set vis[v]  $\leftarrow$  false for all  $v$ ;
Set all  $L_i$  for  $i = 1$  to  $n - 1$  to  $\emptyset$ ;
 $L_0 = s$ ;
vis[s]  $\leftarrow$  true;
for  $i = 0$  to  $n - 1$  do
    if  $L_i = \emptyset$  then
         $\perp$  exit
    while  $L_i \neq \emptyset$  do
         $u \leftarrow L_i.pop()$ ;
         $\backslash\backslash$  In the loop below, replace  $N$  with  $N_{out}$  for a directed graph.;
        foreach  $x \in N(u)$  do
            if vis[ $u$ ] is false then
                vis[ $u$ ]  $\leftarrow$  true;
                 $L_{i+1}.insert(x)$ ;
                p( $x$ )  $\leftarrow$   $u$ ;

```

3.1 Runtime Analysis

We will now look at the runtime for our BFS algorithm (Algorithm 5) for a graph with n nodes and m edges. All of the initialization above the first for loop runs in $O(n)$ time. Visiting each node within the while loop takes $O(1)$ time per node visited. Everything inside the inner foreach loop takes $O(1)$ time per edge scanned, which we can simplify to a runtime of $O(m)$ time overall for the entire inner for loop.

Overall, we see that our runtime is $O(\# \text{ nodes visited} + \# \text{ edges scanned}) = O(m + n)$.

3.2 Correctness

We will now show that BFS correctly computes the shortest path between the source node and all other nodes in the graph. Recall that L_i is the set of nodes that BFS calculates to be distance i from the source node.

Claim 1. For all i , $L_i = \{x | d(s, x) = i\}$.

Proof of Claim 1. We will prove this by (strong) induction on i . Base case ($i = 0$): $L_0 = s$.

Suppose that $L_j = \{x | d(s, x) = j\}$ for every $j \leq i$ (induction hypothesis for i).

We will show two things: (1) if y was added to L_{i+1} , then $d(s, y) = i + 1$, and (2) if $d(s, y) = i + 1$, then y is added to L_{i+1} . After proving (1) and (2) we can conclude that $L_{i+1} = \{y | d(s, y) = i + 1\}$ and complete the induction.

Let's prove (1). First, if y is added to L_{i+1} , it was added by traversing an edge (x, y) where $x \in L_i$, so that there is a path from s to y taking the shortest path from s to x followed by the edge (x, y) , and so $d(s, y) \leq d(s, x) + 1$. Since $x \in L_i$, by the induction hypothesis, $d(s, x) = i$, so that $d(s, y) \leq i + 1$. However, since $y \notin L_j$ for any $j \leq i$, by the induction hypothesis, $d(s, y) > i$, and so $d(s, y) = i + 1$.

Let's prove (2). If $d(s, y) = i + 1$, then by the inductive hypothesis $y \notin L_j$ for $j \leq i$. Let x be the node before y on the $s \rightarrow y$ shortest path P . As $d(s, y) = i + 1$ and the portion of P from s to x is a shortest path and has length exactly i . Thus, by the induction hypothesis, $x \in L_i$. Thus, when x was scanned, edge (x, y) was scanned as well. If y had not been visited when (x, y) was scanned, then y will be added to L_{i+1} . Hence assume that y was visited before (x, y) was scanned. However, since $y \notin L_j$ for any $j \leq i$, y must have been visited by scanning another edge out of a node from L_i , and hence again y is added to L_{i+1} . \square

3.3 BFS versus DFS

If you simplify BFS and DFS to the basics, ignoring all timestamps and levels that we would usually create, BFS and DFS have a very similar structure. Breadth first search explores the nodes closest and then moves outwards, so we can use a queue (first in first out data structure) to put new nodes at the end of the list and pull the oldest/nearest nodes from the top of the list. Depth first search goes as far down a path as it can before coming back to explore other options, so we can use a stack (last in first out data structure) which pushes new nodes on the top and also pulls the newest nodes from the top. See the pseudocode below for more detail.

Algorithm 6: DFS(s) $\setminus \setminus$ s is the source node

```

 $T \leftarrow$  stack
push  $s$  onto  $T$ 
while  $T$  is not empty do
     $u \leftarrow$  pop from top of  $T$ 
    push all unvisited neighbors of  $u$  on top of stack  $T$ 

```

Algorithm 7: BFS(s) $\setminus \setminus$ s is the source node

```

 $T \leftarrow$  queue
push  $s$  onto  $T$ 
while  $T$  is not empty do
     $u \leftarrow$  pop from front of  $T$ 
    push all unvisited neighbors of  $u$  on back of queue  $T$ 

```

1 Connected components in undirected graphs

A **connected component** of an undirected graph $G = (V, E)$ is a maximal set of vertices $S \subset V$ such that for each $u \in S$ and $v \in S$, there exists a path in G from vertex u to vertex v .

Definition 1.1 (Formal Definition) *Let $u \sim v$ if and only if G has a path from vertex u to vertex v . This is an equivalence relation (it is symmetric, reflexive, and transitive). Then, a connected component of G is an equivalence class of this relation \sim . Recall that the equivalence class of a vertex u over a relation \sim is the set of all vertices v such that $u \sim v$.*

1.1 Algorithm to find connected components in a undirected graph

In order to find a connected component of an undirected graph, we can just pick a vertex and start doing a search (BFS or DFS) from that vertex. All the vertices we can reach from that vertex compose a single connected component. To find all the connected components, then, we just need to go through every vertex, finding their connected components one at a time by searching the graph. Note however that we do not need to search from a vertex v if we have already found it to be part of a previous connected component. Hence, if we keep track of what vertices we have already encountered, we will only need to perform one BFS for each connected component.

Proof. When searching from a particular vertex v , we will clearly never reach any nodes outside the connected component with DFS or BFS. So we just need to prove that we will in fact reach all connected vertices. We can prove this by induction: Consider the vertices at minimum distance i from vertex v . Call these vertices “level i ” vertices. If BFS or DFS successfully reaches all vertices at level i , then they must reach all vertices at level $i + 1$, since each vertex at distance $i + 1$ from v must be connected to some vertex at distance i from v . This is the inductive step, and for the base case, DFS or BFS will clearly reach all vertices at level 0 (just v itself). So indeed this algorithm will find each connected component correctly. ■

The searches in the above algorithm take total time $O(|E| + |V|)$, because each BFS or DFS call takes linear time in the number of edges and vertices for its component, and each component is only searched once, so all searches will take time linear in the total number of edges and vertices.

2 Connectivity in directed graphs

How can we extend the notion of connected components to directed graphs?

Definition 2.1 (Strongly connected component (SCC)) *A strongly connected component in a directed graph $G = (V, E)$ is a maximal set of vertices $S \subset V$ such that each vertex $v \in S$ has a path to each other vertex $u \in S$. This is the same as the definition using equivalence classes for undirected graphs, except now $u \sim v$ if and only if there is a path from u to v AND a path from v to u .*

Definition 2.2 (Weakly connected component) *Let $G = (V, E)$ be a directed graph, and let G' be the undirected graph that is formed by replacing each directed edge of G with an undirected edge. Then the weakly connected components of G are exactly the connected components of G' .*

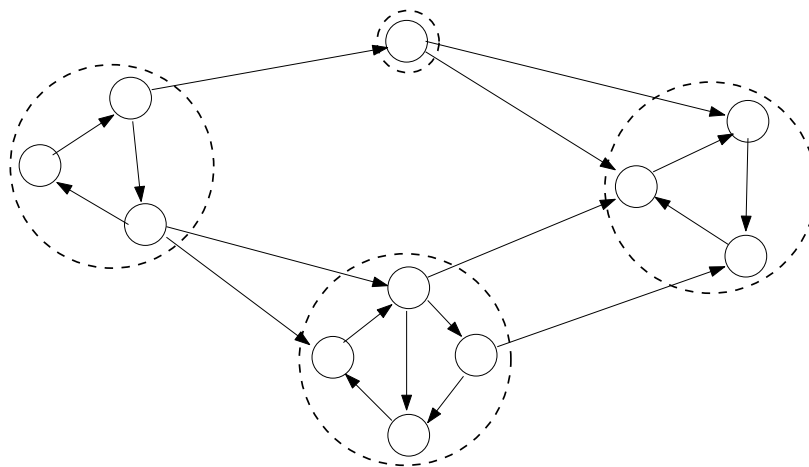


Figure 1: The strongly connected components of a directed graph.

3 Algorithm to find strongly connected components of a directed graph

The algorithm we present is essentially two passes of depth-first search, plus some extremely clever additional book-keeping. The algorithm is described in a top-down fashion in Figures 2–4. Figure 2 describes the top level of the algorithm, and Figures 3 and 4 describe the subroutines DFS-LOOP and DFS. Read these procedures carefully before proceeding to the next section.

Input: a directed graph $G = (V, E)$, in adjacency list representation. Assume that the vertices V are labeled $1, 2, 3, \dots, n$.

1. Let G^{rev} denote the graph G after the orientation of all arcs have been reversed.
2. Run the DFS-LOOP subroutine on G^{rev} , processing vertices in any arbitrary order, to obtain a finishing time $f(v)$ for each vertex $v \in V$.
3. Run the DFS-LOOP subroutine on G , processing vertices in decreasing order of $f(v)$, to assign a “leader” to each vertex $v \in V$. The leader of a vertex v will be the source vertex that the DFS that discovered v started from.
4. The strongly connected components of G correspond to vertices of G that share a common leader.

Figure 2: The top level of our SCC algorithm. The f -values and leaders are computed in the first and second calls to DFS-LOOP, respectively (see below).

NOTE: The algorithm in Figure 2 is a bit different than the one in CLRS/Lecture! (It agrees with the textbook chapter linked at the bottom of these notes). The difference is that in these notes, we first run DFS on the reversed graph, and then we run it again on the original; in CLRS, we first run DFS on the original, and then the second time on the reversed graph. Is it the case that one of these two textbooks has messed it up? In fact, it doesn’t matter: the SCCs of G are the same as the SCCs of G^{rev} , so both algorithms find exactly the same SCC decomposition.

As we’ve seen, each invocation of DFS-LOOP can be implemented in linear time (i.e., $O(|E| + |V|)$), so this whole algorithm will take linear time (the bookkeeping of leaders and finishing times just adds a constant number of operations per each node).

Input: a directed graph $G = (V, E)$, in adjacency list representation.

1. Initialize a global variable t to 0.
[This keeps track of the number of vertices that have been fully explored.]
2. Initialize a global variable s to NULL.
[This keeps track of the vertex from which the last DFS call was invoked.]
3. For $i = n$ downto 1:

[In the first call, vertices are labeled $1, 2, \dots, n$ arbitrarily. In the second call, vertices are labeled by their $f(v)$ -values from the first call.]
 - (a) if i not yet explored:
 - i. set $s := i$ [Set the current source s to i . All vertices discovered from the below DFS call will have their leader set to s .]
 - ii. DFS(G, i)

Figure 3: The DFS-LOOP subroutine.

Input: a directed graph $G = (V, E)$, in adjacency list representation, and a source vertex $i \in V$.

1. Mark i as explored.
[It remains explored for the entire duration of the DFS-LOOP call.]
2. Set $\text{leader}(i) := s$
3. For each arc $(i, j) \in G$:
 - (a) if j not yet explored:
 - i. DFS(G, j)
4. $t++$
5. Set $f(i) := t$

Figure 4: The DFS subroutine. The f -values only need to be computed during the first call to DFS-LOOP, and the leader values only need to be computed during the second call to DFS-LOOP.

4 An Example

But why on earth should this algorithm work? An example should increase its plausibility (though it certainly doesn't constitute a proof of correctness). Figure 5(a) displays a reversed graph G^{rev} , with its vertices numbered arbitrarily, and the f -values computed in the first call to DFS-LOOP. In more detail, the first DFS is initiated at node 9. The search must proceed next to node 6. DFS then has to make a choice between two different adjacent nodes; we have shown the f -values that ensue when DFS visits node 3 before node 8.¹ When DFS visits node 3 it gets stuck; at this point node 3 is assigned a finishing time of 1. DFS backtracks to node 6, proceeds to node 8, then node 2, and then node 5. DFS then backtracks all the way back to node 9, resulting in nodes 5, 2, 8, 6, and 9 receiving the finishing times 2, 3, 4, 5, and 6, respectively. Execution returns to DFS-LOOP, and the next (and final) call to DFS begins at node 7.

Figure 5(b) shows the original graph (with all arcs now unreversed), with nodes labeled with their finishing times. The magic of the algorithm is now evident, as the SCCs of G present themselves to us in order: since we call DFS on the nodes in decreasing order of their finishing times, the first call to DFS discovers the nodes 7–9 (with leader 9); the second the nodes 1, 5, and 6 (with leader 6); and the third the remaining three nodes (with leader 4).

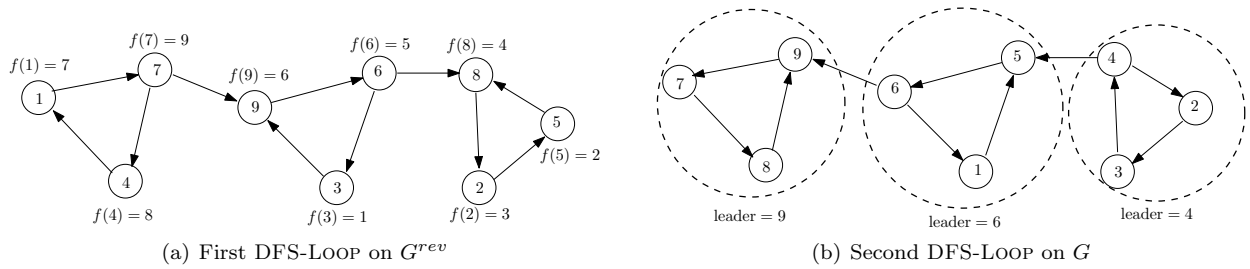


Figure 5: Example execution of the strongly connected components algorithm. In (a), nodes are labeled arbitrarily and their finishing times are shown. In (b), nodes are labeled by their finishing times and their leaders are shown.

5 Proof of Correctness

5.1 The Acyclic Meta-Graph of SCCs

First, observe that the strongly connected components of a directed graph form an acyclic “meta-graph”, where the meta-nodes correspond to the SCCs C_1, \dots, C_k , and there is an arc $C_h \rightarrow C_\ell$ with $h \neq \ell$ if and only if there is at least one arc (i, j) in G with $i \in C_h$ and $j \in C_\ell$. This directed graph must be acyclic: since within a SCC you can get from anywhere to anywhere else on a directed path, in a purported directed cycle of SCCs you can get from every node in a constituent SCC to every other node of every other SCC in the cycle. Thus the purported cycle of SCCs is actually just a single SCC. Summarizing, every directed graph has a useful “two-tier” structure: zooming out, one sees a DAG (Directed Acyclic Graph) on the SCCs of the graph; zooming in on a particular SCC exposes its finer-grained structure. For example, the meta-graphs corresponding to the directed graphs in Figures 1 and 5(b) are shown in Figure 6.

5.2 The Key Lemma

Correctness of the algorithm hinges on the following key lemma.

Key Lemma: Consider two “adjacent” strongly connected components of a graph G : components C_1 and C_2 such that there is an arc (i, j) of G with $i \in C_1$ and $j \in C_2$. Let $f(v)$ denote the finishing time of

¹Different choices of which node to visit next generate different sets of f -values, but our proof of correctness will apply to all ways of resolving these choices.

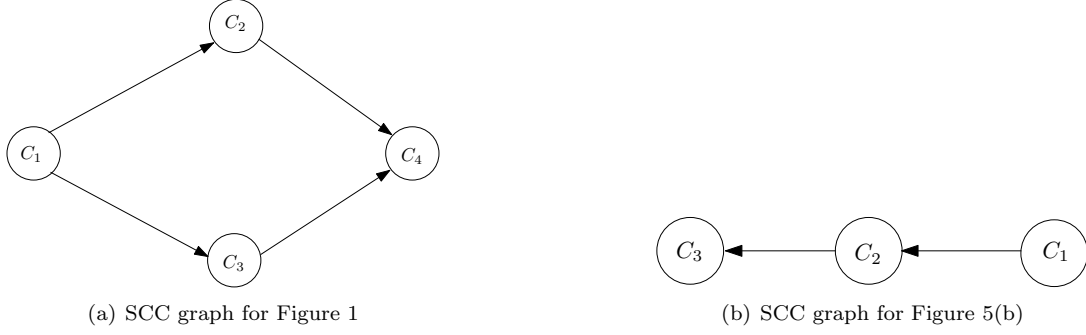


Figure 6: The DAGs of the SCCs of the graphs in Figures 1 and 5(b), respectively.

vertex v in some execution of DFS-LOOP on the reversed graph G^{rev} . Then

$$\max_{v \in C_1} f(v) < \max_{v \in C_2} f(v).$$

Proof of Key Lemma: Consider two adjacent SCCs C_1 and C_2 , as they appear in the reversed graph G^{rev} — where there is an arc (j, i) , with $j \in C_2$ and $i \in C_1$ (Figure 7). Because the equivalence relation defining the SCCs is symmetric, G and G^{rev} have the same SCCs; thus C_1 and C_2 are also SCCs of G^{rev} . Let v denote the first vertex of $C_1 \cup C_2$ visited by DFS-LOOP in G^{rev} . There are now two cases.

First, suppose that $v \in C_1$ (Figure 7(a)). Since there is no non-trivial cycle of SCCs (Section 5.1), there is no directed path from v to C_2 in G^{rev} . Since DFS discovers everything reachable and nothing more, it will finish exploring all vertices in C_1 without reaching any vertices in C_2 . Thus, *every* finishing time in C_1 will be smaller than *every* finishing time in C_2 , and this is even stronger than the assertion of the lemma. (Cf., the left and middle SCCs in Figure 5.)

Second, suppose that $v \in C_2$ (Figure 7(b)). Since DFS discovers everything reachable and nothing more, the call to DFS at v will finish exploring all of the vertices in $C_1 \cup C_2$ before ending. Thus, the finishing time of v is the largest amongst vertices in $C_1 \cup C_2$, and in particular is larger than all finishing times in C_1 . (Cf., the middle and right SCCs in Figure 5.) This completes the proof.

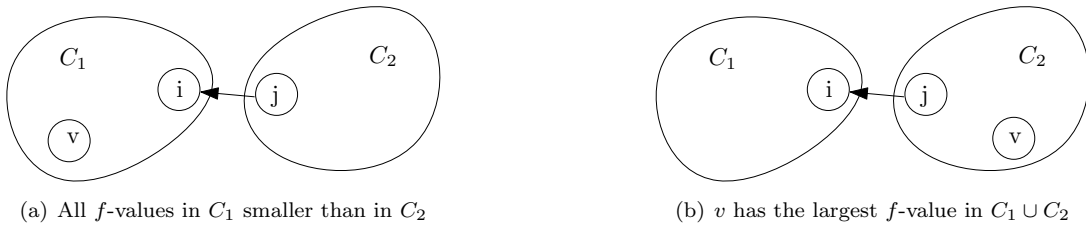


Figure 7: Proof of Key Lemma. Vertex v is the first in $C_1 \cup C_2$ visited during the execution of DFS-LOOP on G^{rev} .

5.3 The Final Argument

The Key Lemma says that traversing an arc from one SCC to another (in the original, unreversed graph) strictly increases the maximum f -value of the current SCC. For example, if f_i denotes the largest f -value of a vertex in C_i in Figure 6(a), then we must have $f_1 < f_2, f_3 < f_4$. Intuitively, when DFS-LOOP is invoked on G , processing vertices in decreasing order of finishing times, the successive calls to DFS peel off the SCCs of the graph one at a time, like layers of an onion.

We now formally prove correctness of our algorithm for computing strongly connected components. Consider the execution of DFS-LOOP on G . We claim that whenever DFS is called on a vertex v , the vertices explored — and assigned a common leader — by this call are precisely those in v 's SCC in G . Since DFS-LOOP eventually explores every vertex, this claim implies that the SCCs of G are precisely the groups of vertices that are assigned a common leader.

We proceed by induction. Let S denote the vertices already explored by previous calls to DFS (initially empty). Inductively, the set S is the union of zero or more SCCs of G . Suppose DFS is called on a vertex v and let C denote v 's SCC in G . Since the SCCs of a graph are disjoint, S is the union of SCCs of G , and $v \notin S$, no vertices of C lie in S . Thus, this call to DFS will explore, at the least, all vertices of C . By the Key Lemma, every outgoing arc (i, j) from C leads to some SCC C' that contains a vertex w with a finishing time larger than $f(v)$. Since vertices are processed in decreasing order of finishing time, w has already been explored and belongs to S ; since S is the union of SCCs, it must contain all of C' . Summarizing, every outgoing arc from C leads directly to a vertex that has already been explored. Thus this call to DFS explores the vertices of C and nothing else. This completes the inductive step and the proof of correctness.

6 Another resource

Additional reference for another treatment of strongly connected components in directed graphs:
<https://people.eecs.berkeley.edu/~vazirani/algorithms/chap3.pdf>

1 Dijkstra's Algorithm

Now we will solve the single source shortest paths problem in graphs with nonnegative weights using Dijkstra's algorithm. The key idea, that Dijkstra will maintain as an invariant, is that $\forall t \in V$, the algorithm computes an estimate $d[t]$ of the distance of t from the source such that:

1. At any point in time, $d[t] \geq d(s, t)$, and
2. when t is finished, $d[t] = d(s, t)$.

Algorithm 1: Dijkstra($G = (V, E), s$)

```

 $\forall t \in V, d[t] \leftarrow \infty$  // set initial distance estimates
 $d[s] \leftarrow 0$ 
 $F \leftarrow \{v \mid \forall v \in V\}$  //  $F$  is set of nodes that are yet to achieve final distance estimates
 $D \leftarrow \emptyset$  //  $D$  will be set of nodes that have achieved final distance estimates
while  $F \neq \emptyset$  do
     $x \leftarrow$  element in  $F$  with minimum distance estimate
    for  $(x, y) \in E$  do
         $d[y] \leftarrow \min\{d[y], d[x] + w(x, y)\}$  // "relax" the estimate of  $y$ 
        // to maintain paths: if  $d[y]$  changes, then  $\pi(y) \leftarrow x$ 
     $F \leftarrow F \setminus \{x\}$ 
     $D \leftarrow D \cup \{x\}$ 

```

We will prove that Dijkstra correctly computes the distances from s to all $t \in V$.

Claim 1. For every u , at any point of time $d[u] \geq d(s, u)$.

A formal proof of this claim proceeds by induction. In particular, one shows that at any point in time, if $d[u] < \infty$, then $d[u]$ is the weight of some path from s to u . Thus at any point $d[u]$ is at least the weight of the *shortest* path, and hence $d[u] \geq d(s, u)$.

As a base case, we know that $d[s] = 0 = d(s, s)$ and all other distance estimates are $+\infty$, so we know that the claim holds initially. Now, when $d[u]$ is changed to $d[x] + w(x, u)$ then (by the induction hypothesis) there is a path from s to x of weight $d[x]$ and an edge (x, u) of weight $w(x, u)$. This means there is a path from s to u of weight $d[u] = d[x] + w(x, u)$. This implies that $d[u]$ is at least the weight of the shortest path $= d(s, u)$, and the induction argument is complete.

Claim 2. When node x is placed in D , $d[x] = d(s, x)$.

Notice that proving the above claim is sufficient to prove the correctness of the algorithm since $d[x]$ is never changed again after x is added to D : the only way it could be changed is if for some node $y \in F$, $d[y] + w(y, x) < d[x]$ but this can't happen since $d[x] \leq d[y]$ and $w(y, x) \geq 0$ (all edge weights are nonnegative). The assertion $d[x] \leq d[y]$ for all $y \in F$ stays true at all points after x is inserted into D : assume for contradiction that at some point for some $y \in F$ we get $d[y] < d[x]$ and let y be the first such y . Before $d[y]$ was updated $d[y'] \geq d[x]$ for all $y' \in F$. But then when $d[y]$ was changed, it was due to some neighbor y' of y in F , but $d[y'] \geq d[x]$ and all weights are nonnegative, so we get a contradiction

We prove this claim by induction on the order of placement of nodes into D . For the base case, s is placed into D where $d[s] = d(s, s) = 0$, so initially, the claim holds.

For the inductive step, we assume that for all nodes y currently in D , $d[y] = d(s, y)$. Let x be the node that currently has the minimum distance estimate in F (this is the node about to be moved from F to D). We will show that $d[x] = d(s, x)$ and this will complete the induction.

Let p be a shortest path from s to x . Suppose z is the node on p closest to x for which $d[z] = d(s, z)$. We know z exists since there is at least one such node, namely s , where $d[s] = d(s, s)$. By the choice of z , for every node y on p between z (not inclusive) to x (inclusive), $d[y] > d(s, y)$. Consider the following options for z .

1. If $z = x$, then $d[x] = d(s, x)$ and we are done.
2. Suppose $z \neq x$. Then there is a node z' after z on p . (Here it is possible that $z' = x$.) We know that $d[z] = d(s, z) \leq d(s, x) \leq d[x]$. The first \leq inequality holds because subpaths of shortest paths are shortest paths as well, so that the prefix of p from s to z has weight $d(s, z)$. In addition, the weights on edges are non-negative, so that the portion of p from z to x has a nonnegative weight, and so $d(s, z) \leq d(s, x)$. The subsequent \leq holds by Claim 1. We know that if $d[z] = d[x]$ all of the previous inequalities are equalities and $d[x] = d(s, x)$ and the claim holds.

Finally, towards a contradiction, suppose $d[z] < d[x]$. By the choice of $x \in F$ we know $d[x]$ is the minimum distance estimate that was in F . Thus, since $d[z] < d[x]$, we know $z \notin F$ and must be in D , the finished set. This means the edges out of z , and in particular (z, z') , were already relaxed by our algorithm. But this means that $d[z'] \leq d(s, z) + w(z, z') = d(s, z')$, because z is on the shortest path from s to z' , and the distance estimate of z' must be correct. However, this contradicts z being the closest node on p to x meeting the criteria $d[z] = d(s, z)$. Thus, our initial assumption that $d[z] < d[x]$ must be false and $d[x]$ must equal $d(s, x)$.

1.1 Implementation of Dijkstra's Algorithm

Consider implementing Dijkstra's algorithm with a priority queue to store the set F , where the distance estimates are the keys. The initialization step takes $O(n)$ operations to set n distance estimate values to infinity and 0. In each iteration of the while loop, we make a call to find the node x in F with the minimum distance estimate (via, say, **FindMin** operation). Then, we relax each edge leaving x (via **DecreaseKey**). We remove node x (via **DeleteMin**) and add it to D . In total, there are n calls to **FindMin** and n calls to **DeleteMin** since nodes are never re-inserted into F . Similarly, there will be m calls to **DecreaseKey** to relax the edges since each edge will be relaxed at most once.

Depending on how quickly our priority queue can support **FindMin**, **DeleteMin**, and **DecreaseKey** operations, the total runtime of Dijkstra's algorithm is on the order of

$$n \cdot (T_{\text{FindMin}}(n) + T_{\text{DeleteMin}}(n)) + m \cdot T_{\text{DecreaseKey}}(n).$$

We consider the following implementations of the priority queue for storing F :

- Store F as an array:
Each slot corresponds to a node and stores the distance $d[j]$ if $j \in F$, or **NIL** otherwise. **DecreaseKey** runs in $O(1)$ as nodes are indexed. **FindMin** and **DeleteMin** run in $O(n)$ as the array is not sorted and we have to go through the whole array. The total runtime is $O(m + n^2) = O(n^2)$.
- Store F as a red-black tree:
All operations run in $O(\log n)$ time. We implement **DecreaseKey** by deleting and re-inserting with the new key. The total runtime is $O((m + n) \log n)$. If graph G is sparse with few edges, then the red-black tree implementation is faster than the array implementation. However, it can be slower when G is dense with $m = \Theta(n^2)$.

- Store F as a Fibonacci heap:

Fibonacci heaps are a complex data structure which is able to support the operations **Insert** in $O(1)$, **FindMin** in $O(1)$, **DecreaseKey** in $O(1)$ and **DeleteMin** in $O(\log n)$ “amortized” time, over a sequence of calls to these operations. The meaning of amortized time in this case is as follows: starting from an empty Fibonacci heap, any sequence of operations that includes a **Insert**’s, b **FindMin**’s, c **DecreaseKey**’s and d **DeleteMin**’s take $O(a + b + c + d \log n)$ time. The total runtime is $O(m + n \log n)$.

To conclude, Dijkstra’s algorithm can be very fast when implemented the right way! However, it has a few drawbacks:

- It doesn’t work with negative edge weights: we used the fact that the weights were non-negative a few times in the correctness proof above.
- It’s not very amenable to frequent updates. Suppose that you had already run Dijkstra’s algorithm from a particular point, but one weight in the graph changed. How would you recover from this? Next time, we’ll see the Bellman-Ford algorithm, which can be better on both of these fronts.

2 Negative Edge Weights

Note that Dijkstra’s algorithm solves the single source shortest paths problem when there are no edges with negative weights. While Dijkstra’s algorithm may fail on certain graphs with negative edge weights, having a negative cycle (i.e., a cycle in the graph for which the sum of edge weights is negative) is a bigger problem for any shortest path algorithm. When computing a shortest path between two vertices, each additional traversal along the cycle lowers the overall cost incurred and an arbitrarily small distance can be reached after looping around the cycle multiple times. In this case, the shortest path to a node on the cycle is not well defined since it is (negatively) infinite.

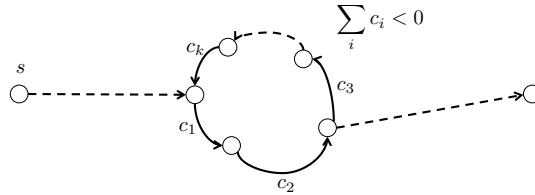


Figure 1: Assume there is a negative cycle along the $s - t$ path. The distance between s and t is not well-defined.

For example, consider the graph in Figure 1. The shortest path from s to t would start from the node s , loop around the negative cycle an infinite number of times and eventually reach destination t . The shortest path would, hence, be of infinite length and is not well-defined.

Besides the negative cycles, there are no problems in computing the shortest paths in a graph with negative edge weights. In fact, there are many applications where allowing negative edge weights is important.

3 Bellman-Ford Algorithm

In this section, we study the Bellman-Ford algorithm that solves the single source shortest paths problem on graphs with edges with potentially negative weights. Given a directed graph $G = (V, E)$ with edge weights given by $c(x, y)$ for $(x, y) \in E$, we want to compute the shortest path distances $d(s, v)$ from source s for all $v \in V$. More specifically, the Bellman-Ford algorithm:

- Detects a negative cycle if it exists and is reachable from s , or

- Computes the shortest path distances $d(s, v)$ for all $v \in V$.

Algorithm 2: Bellman-Ford Algorithm

```

 $d[v] \leftarrow \infty, \forall v \in V$  // set initial distance estimates
// to maintain paths: set  $\pi(v) \leftarrow \text{nil}$  for all  $v$ ,  $\pi(v)$  represents the predecessor of  $v$ 
 $d[s] \leftarrow 0$  // set distance to start node trivially as 0
for  $i$  from 1  $\rightarrow n - 1$  do
    for  $(u, v) \in E$  do
         $d[v] \leftarrow \min\{d[v], d[u] + w(u, v)\}$  // update the distance estimate for  $v$ 
        // to maintain paths - if  $d[v]$  changes, then  $\pi(v) \leftarrow u$ 
// Negative Cycle Step
for  $(u, v) \in E$  do
    if  $d[v] > d[u] + w(u, v)$  then
        return "Negative Cycle"; // negative cycle detected
return  $d[v] \forall v \in V$ 

```

Note $\pi(\cdot)$ is used to store the shortest paths found and $\pi(v)$ represents the predecessor of v on the shortest path from s to v .

NOTE: This version of Bellman-Ford is a bit different than the one we presented in class! As mentioned in class, we changed it up slightly to be more in line with the next lecture on Dynamic Programming. However, the analysis is basically the same. We'll analyze the above version here.

For an example run of the Bellman-Ford algorithm, please refer to the lecture slides or CLRS.

The total runtime of the Bellman-Ford algorithm is $O(mn)$. In the first for loop, we repeatedly update the distance estimates $n - 1$ times on all m edges in time $O(mn)$. In the second for loop, we go through all m edges to check for negative cycles in time of $O(m)$.

We prove the correctness of the Bellman-Ford algorithm in two steps:

Claim 3. *If there is a negative cycle reachable from s , then the Bellman-Ford algorithm detects and reports "Negative Cycles".*

Proof. For the sake of contradiction, suppose there exists a negative cycle C reachable from the source s and the Bellman-Ford algorithm does not report "Negative Cycles". Assume C contains nodes v_1, v_2, \dots, v_k with edges (v_i, v_{i+1}) for $i = 1, \dots, k$ such that $\sum_{i=1}^k c(v_i, v_{i+1}) < 0$, where $v_{k+1} = v_1$. See Figure 2. Let $d[\cdot]$ be the distance estimates determined in the first for loop of the algorithm.

Since C is reachable from s , there is a path from s to v_1 and to all nodes on C . In particular, there exist simple paths, i.e., paths without cycles, of at most $n - 1$ edges to the nodes of C . In the first for loop, the edges on each such simple path get relaxed in order and consequently, $d[v_i]$ will be some finite number less than ∞ for $i = 1, \dots, k$. Since the Bellman-Ford algorithm does not report "Negative Cycles" in the second for loop, it must be that $d[v_{i+1}] \leq d[v_i] + c(v_i, v_{i+1})$ for $i = 1, \dots, k$. Adding the inequalities, we obtain

$$\sum_{i=1}^k d[v_{i+1}] \leq \sum_{i=1}^k d[v_i] + \sum_{i=1}^k c(v_i, v_{i+1}) .$$

As we are summing over the cycle C , the terms $\sum_{i=1}^k d[v_{i+1}]$ and $\sum_{i=1}^k d[v_i]$ are equal and can be cancelled. It follows that $0 \leq \sum_{i=1}^k c(v_i, v_{i+1})$. This contradicts that C is a negative cycle. □

In the next claim, we show that if the graph has no negative cycles reachable from the source, then the Bellman-Ford algorithm returns the correct shortest path distances.

Claim 4. *If G has no negative cycles reachable from s , then $d[v] = d(s, v), \forall v \in V$.*

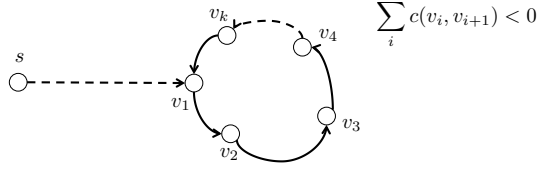


Figure 2: A negative cycle reachable from source s

Proof. Let $d_k(v)$ be the value of $d[v]$ after k iterations of the first for loop. We prove by induction the statement that $d_k(v)$ is at most the minimum distance of a path from s to v with at most k edges. Then, we will have $d_{n-1}(v) = d[v]$ for all node v at termination. We'll argue below that if there is any path from s to v , then there is some shortest path with at most $n - 1$ edges, so this means

$$\text{dist}(s, v) \leq d[v] = d_{n-1}(v) \leq \text{minimum cost of a path with at most } n - 1 \text{ edges} = \text{dist}(s, v).$$

Thus, everything in the above inequality chain is equal, and in particular $d[v]$ is equal to the distance from s to v . Above, we used the fact that $d[v]$ is an over-estimate on $\text{dist}(s, v)$, which follows from our analysis of Dijkstra's algorithm.

We now argue that if there is a path from s to v , then there exists a shortest path from s to v has at most $n - 1$ edges. If a shortest path has a cycle, the cycle cannot be negative and we can remove it and improve its total distance. If the cycle has a positive weight, removing the cycle will strictly improve the shortest path's distance. If the cycle has zero weight, we can ignore the cycle. Hence, we can assume that shortest paths are simple, that is, do not have cycles.

Base Case: When $k = 0$, the distance estimates have been just initialized. So, $d_0(v) = \infty$ if $v \neq s$. Furthermore, $d_0(s) = 0 = d(s, s)$, which is the minimum distance of length-0 paths from s to s . The statement is satisfied for the base case.

Inductive Step: Assume that $d_{k-1}(v)$ is at most the minimum distance of a $s \rightarrow v$ path on at most $k - 1$ edges for all v .

Consider $v \neq s$. Let P be a shortest simple $s \rightarrow v$ path on at most k edges. Let u be the node just before v on P , and let Q be the sub-path of P from s to u . The path Q would have at most $k - 1$ edges and is a shortest path from s to u with at most $k - 1$ edges, since sub-paths of shortest paths are also shortest paths. By the inductive hypothesis, Q has cost at most $d_{k-1}(u)$.

In the k -th iteration, we update $d_k(v)$ such that $d_k(v) \leq d_{k-1}(u) + w(u, v) = w(Q) + w(u, v) = w(P)$.

The induction is complete, and the claim is proved. \square

1 More on the Bellman-Ford Algorithm

We didn't quite make it to the Bellman-Ford algorithm last week, so we'll re-hash some of that again today. Last week we introduced Bellman-Ford in the context of Dijkstra's algorithm. We'll see it in this lecture in a different way, so as to naturally introduce *dynamic programming*. The Bellman-Ford algorithm is a dynamic programming algorithm, and dynamic programming is a basic paradigm in algorithm design used to solve problems by relying on intermediate solutions to smaller subproblems. The main step for solving a dynamic programming problem is to analyze the problem's optimal substructure and overlapping subproblems.

The Bellman-Ford algorithm is pretty simple to state:

Algorithm 1: Bellman-Ford Algorithm (G, s)

```

 $d^{(0)}[v] = \infty \forall v \in V$ 
 $d^{(0)}[s] = 0$ 
 $d^{(k)}[v] = \text{None} \forall v \in V \forall k > 0$ 
for  $k = 1, \dots, n - 1$  do
     $d^{(k)}[v] \leftarrow d^{(k-1)}[v]$ 
    for  $(u, v) \in E$  do
         $d^{(k)}[v] \leftarrow \min\{d^{(k)}[v], d^{(k-1)}[u] + w(u, v)\}$ 
    // here we can release the memory for  $d^{(k-1)}$ , we'll never need it again.
return  $d^{(n)}[v], \forall v \in V$ 

```

What's going on here? The value $d^{(k)}[v]$ is the cost of the shortest path from s to v with at most k edges in it. Once we realize this, a proof by induction (similar to the one in Lecture Notes 11) falls right out, with the inductive hypothesis that " $d^{(k)}[v]$ is the cost of the shortest path from s to v with at most k edges in it."

Runtime and Storage. The runtime of the Bellman-Ford algorithm is $O(mn)$; for n iterations, we loop through all the edges. This is slower than Dijkstra's algorithm. However, it is simpler to implement, and further as we saw in Lecture Notes 11.5, it can handle negative edge weights. For storage, in the pseudocode above, we keep n different arrays $d^{(k)}$ of length n . This isn't necessary: we only need to store two of them at a time. This is noted in the comment in the pseudocode.

1.1 What's really going on here?

The thing that makes that Bellman-Ford algorithm work is that that the shortest paths of length at most k can be computed by leveraging the shortest paths of length at most $k - 1$. More specifically, we relied on the following recurrence relation between the intermediate solutions:

$$d^{(k)}[v] = \min_{u \in V} \left\{ d^{(k-1)}[u] + w(u, v) \right\}$$

where $d_k[v]$ is the length of the shortest path from source s to node v using at most k edges, and $w(u, v)$ is the weight of edge (u, v) . (Above, we are assuming $w(v, v) = 0$).

This idea of using the intermediate solutions is similar to the divide-and-conquer paradigm. However, a divide-and-conquer algorithm recursively computes intermediate solutions once for each subproblem, but a dynamic programming algorithm solves the subproblems exactly once and uses these results multiple times.

2 Dynamic Programming

The idea of dynamic programming is to have a table of solutions of subproblems and fill it out in a particular order (e.g. left to right and top to bottom) so that the contents of any particular table cell only depends on the contents of cells before it. For example, in the Bellman-Ford algorithm, we filled out $d^{(k-1)}$ before we filled out $d^{(k)}$; and in order to fill out $d^{(k)}$, we just had to look back at $d^{(k-1)}$, rather than compute anything new.

In this lecture, we will discuss dynamic programming more, and also see another example: the Floyd-Warshall algorithm.

2.1 Dynamic Programming Algorithm Recipe

Here, we give a general recipe for solving problems (usually optimization problems) by dynamic programming. Dynamic programming is a good candidate paradigm to use for problems with the following properties:

- Optimal substructure gives a recursive formulation; and
- Overlapping subproblems give a small table, that is, we can store the precomputed answers such that it doesn't actually take too long when evaluating a recursive function multiple times.

What exactly do these things mean? We'll discuss them a bit more below, with the Bellman-Ford algorithm in mind as a reference.

2.1.1 Optimal Substructure

By this property, we mean that the optimal solution to the problem is composed of optimal solutions to smaller *independent* subproblems.

For example, the shortest path from s to t consists of a shortest path P from s to k (for node k on P) and a shortest path from k to t . This allows us to write down an expression for the distance between s and t with respect to the lengths of sub-paths:

$$d(s, t) = d(s, k) + d(k, t), \text{ for all } k \text{ on a shortest } s - t \text{ path}$$

We used this in the Bellman-Ford algorithm when we wrote

$$d^{(k)}[u] = \min_{v \in V} \{d^{(k-1)}[v] + w(u, v)\}.$$

2.1.2 Overlapping subproblems

The goal of dynamic programming is to construct a table of entries, where early entries in the table can be used to compute later entries. Ideally, the optimal solutions of subproblems can be reused multiple times to compute the optimal solutions of larger problems.

For our shortest paths example, $d(s, k)$ can be used to compute $d(s, t)$ for any t where the shortest $s - t$ path contains k . To save time, we can compute $d(s, k)$ once and just look it up each time, instead of recomputing it.

More concretely in the Bellman-Ford example, suppose that (v, u) and (v, u') are both in E . When we go to compute $d^{(k)}[u]$, we'll need $d^{(k-1)}[v]$. Then when we go to compute $d^{(k)}[u']$, we'll need $d^{(k-1)}[v]$ again. If we just set this up as a divide-and-conquer algorithm, this would be extremely wasteful, and we'd be re-doing lots of work. By storing this value in a table and looking it up when we need it, we are taking advantage of the fact that these subproblems overlap.

2.1.3 Implementations

The above two properties lead to two different ways to implement dynamic programming algorithms. In each, we will store a table T with optimal solutions to subproblems; the two variants differ in how we decide to fill up the table:

1. Bottom-up: Here, we will fill in the table starting with the smallest subproblems. Then, assuming that we have computed the optimal solution to small subproblems, we can compute the answers for larger subproblems using our recursive optimal substructure.
2. Top-down: In this approach, we will compute the optimal solution to the entire problem recursively. At each recursive call, we will end up looking up the answer or filling in the table if the entry has not been computed yet.

In fact, these two methods are completely equivalent. Any dynamic programming algorithm can be formulated as an iterative table-filling algorithm or a recursive algorithm with look-ups.

3 Floyd-Warshall Algorithm

The Floyd-Warshall Algorithm solves the All Pairs Shortest Path (APSP) problem: given a graph G , find the shortest path distances $d(s, t)$ for all $s, t \in V$, and, for the purpose of storing the shortest paths, the predecessor $\pi(s, t)$ which is the node right before t on the s - t shortest path.

Let's speculate about APSP for a moment. Consider the case when the edge weights are nonnegative. We know we can compute APSP by running Dijkstra's algorithm on each node $v \in V$ and obtain a total runtime of $O(mn + n^2 \log n)$. The runtime of the Floyd-Warshall algorithm, on the other hand, is $O(n^3)$. We know that in the worst case $m = O(n^2)$, and thus, the Floyd-Warshall algorithm can be at least as bad as running Dijkstra's algorithm n times! Then why do we care to explore this algorithm? The reason is that the Floyd-Warshall algorithm is very easy to implement compared to Dijkstra's algorithm. The benefit of using simple algorithms is that they can often be extended and in practice can run relatively faster compared to algorithms that may have a huge overhead.

An added benefit of the Floyd-Warshall algorithm is that it also supports negative edge weights, whereas Dijkstra's algorithm does not.¹

As mentioned, the optimum substructure with overlapping subproblems for shortest paths is that for all node k on an s - t shortest path, $d(s, t) = d(s, k) + d(k, t)$. We refine this observation as follows. Suppose that the nodes of the graph are identified with the integers from 1 to n . Then, if k is the maximum node on an s - t shortest path, then $d(s, t) = d(s, k) + d(k, t)$ and moreover, the subpaths from s to k and from k to t only use nodes up to $k - 1$ internally.

We hence get independent subproblems in which we compute $d_k(s, t)$ for all s, t that are the smallest weight of an s - t path that only uses nodes $1, \dots, k$ internally. This motivates the Floyd-Warshall algorithm, Algorithm 2 below (please note that we will refer to the nodes of G by the names $1, \dots, n$).

Correctness when there are no negative cycles In the k -th iteration of the Floyd-Warshall algorithm, $d_k(u, v)$ is the minimum weight of a $u \rightarrow v$ path that uses as intermediate nodes only nodes from $\{1, \dots, k\}$. What does the recurrence relation represent? If P is a shortest path from u to v using $1, \dots, k$ as intermediate nodes, there are two cases. Assume that P is a simple path, since shortest paths are simple when there are no negative cycles:

- *Case 1: P contains k* : In this case, we know that neither the path from u to k nor the path from k to v contains any nodes that are greater than $k - 1$. In this case, we can simply use $d_k(u, v) = d_{k-1}(u, k) + d_{k-1}(k, v)$.

¹Although, one can still use Dijkstra's algorithm n times, if one preprocesses the edge weights initially via something called the Johnson's trick.

Algorithm 2: Floyd-Warshall Algorithm (G)

```
 $d_k(u, u) = 0, \forall u \in V, k \in \{0, \dots, n\}$   
 $d_k(u, v) = \infty, \forall u, v \in V, u \neq v, k \in \{1, \dots, n\}$   
 $d_0(u, v) = c(u, v), \forall (u, v) \in E$   
 $d_0(u, v) = \infty, \forall (u, v) \notin E$   
for  $k = 1, \dots, n$  do  
    for  $(u, v) \in V$  do  
         $d_k(u, v) = \min\{d_{k-1}(u, v), d_{k-1}(u, k) + d_{k-1}(k, v)\}$  // update the estimate of  $d(u, v)$   
return  $d_n(u, v), \forall u, v \in V$ 
```

- *Case 2:* P does not contain k : We can say that $d_k(u, v) = d_{k-1}(u, v)$

We initialize each $d_0(u, v)$ as the edge weight $c(u, v)$ if $(u, v) \in E$, else we set it to ∞ in the bottom-most row in our dynamic programming table. Now, as we increment k to 1, we effectively find the minimum distance path between $u, v \in V$ that go through node 1, and populate the table with the results. We continue this process to find the shortest paths that go through nodes 1 and 2, then 1, 2, and 3 and so on until we find the shortest path through all n nodes.

Negative cycles. The Floyd-Warshall algorithm can be used to detect negative cycles: examine whether $d_n(u, u) < 0$ for any $u \in V$. If there exists u such that $d_n(u, u) < 0$, there is a negative cycle, and if not, then there isn't. The reason for this is that if there is a simple path P from u to u of negative weight (i.e., a negative cycle containing u), then $d_n(u, u)$ will be at most its weight, and hence, will be negative. Otherwise, no path can cause $d_n(u, u)$ to be negative.

Runtime. The runtime of the Floyd-Warshall algorithm is proportional to the size of the table $\{d_i(u, v)\}_{i,u,v}$ since filling each entry of the table only depends on at most two other entries filled in before it. Thus, the runtime is $O(n^3)$.

Space usage. Note that for both the algorithms we covered today, the Floyd-Warshall and Bellman-Ford algorithms, we can choose to store only two rows of the table instead of the complete table in order to save space. This is because the row being populated always depends only on the row right below it. This space saving optimization is not a general property of tables formed as a result of the dynamic programming method, and the slot dependencies in some dynamic programming problems may lie on arbitrary positions on the table thereby forcing us to store the complete table.

A Note on the Longest Path Problem

We discussed the shortest path problem in detail and provided algorithms for a number of variants of the problem. We might equally be interested in computing the longest simple path in a graph. A first approach is to formulate a dynamic programming algorithm. Indeed, consider any path, even the longest, between two nodes s and t . Its length $\ell(s, t)$ equals the sum $\ell(s, k) + \ell(k, t)$ for any node k on the path. However, this does not yield an optimal substructure: in general, neither subpath $s \rightarrow k$, $k \rightarrow t$ would be a longest path, and even if one is a longest path, the other one cannot use any nodes that appear on the first since the longest path is required to be simple. Hence the two subproblems $\ell(s, k)$ and $\ell(k, t)$ are not even independent! It turns out that finding the longest path does not seem to have any optimal substructure, which makes it difficult to avoid exhaustive search through dynamic programming. The longest path problem is actually a very difficult problem to solve and is NP-hard. The best known algorithm for it runs in exponential time.

4 Why is it called dynamic programming?

The name doesn't immediately make a lot of sense. "Dynamic programming" sounds like the type of coding that action heroes do in late-90's hacker movies. However, "programming" here refers to a program, like a plan (for example, the path you are trying to optimize), not to programming a computer. "Dynamic" refers to the fact that we update the table over time: this is a dynamic process. But the fact that it makes you (or at least me) think about action movies isn't an accident. As Richard Bellman, who coined the term, writes in his autobiography:

An interesting question is, Where did the name, dynamic programming, come from? The 1950s were not good years for mathematical research. We had a very interesting gentleman in Washington named Wilson. He was Secretary of Defense, and he actually had a pathological fear and hatred of the word, research. I'm not using the term lightly; I'm using it precisely. His face would suffuse, he would turn red, and he would get violent if people used the term, research, in his presence. You can imagine how he felt, then, about the term, mathematical. The RAND Corporation was employed by the Air Force, and the Air Force had Wilson as its boss, essentially. Hence, I felt I had to do something to shield Wilson and the Air Force from the fact that I was really doing mathematics inside the RAND Corporation. What title, what name, could I choose? In the first place, I was interested in planning, in decision-making, in thinking. But planning, is not a good word for various reasons. I decided therefore to use the word, "programming". I wanted to get across the idea that this was dynamic, this was multistage, this was time-varying. I thought, let's kill two birds with one stone. Let's take a word which has an absolutely precise meaning, namely dynamic, in the classical physical sense. It also has a very interesting property as an adjective, and that is it's impossible to use the word, dynamic, in the pejorative sense. Try thinking of some combination which will possibly give it a pejorative meaning. It's impossible. Thus, I thought dynamic programming was a good name. It was something not even a Congressman could object to. So I used it as an umbrella for my activities.

1 Overview

Last lecture, we talked about dynamic programming (DP), a useful paradigm and one technique that you should immediately consider when you are designing an algorithm. We covered the Bellman-Ford algorithm for solving the single source shortest path problem, and we talked about the Floyd-Warshall algorithm for solving the all pairs shortest path problem.

This lecture, we will cover some more examples of dynamic programming, and start to see a recipe for how to come up with DP solutions. We will talk about three problems today: longest common subsequence, knapsack, and maximum weight independent set in trees.

In general, here are the steps to coming up with a dynamic programming algorithm:

1. **Identify optimal substructure:** how are we going to break up an optimal solution into optimal sub-solutions of sub-problems? We're looking for a way to do this so that there are *overlapping* sub-problems, so that a dynamic programming approach will be effective.
2. **Recursively define the value of an optimal solution:** Write down a recursive formulation of the optimum, in terms of sub-solutions.
3. **Find the optimal value:** Turn this recursive formulation into a dynamic programming algorithm to compute the value of the optimal solution.
4. **Find the optimal solution:** Once we've figured out how to find the cost of the optimal solution, we can go back and figure out how to keep enough information in our algorithm so that we can find the solution itself.
5. **Tweak the implementation:**¹ Often it's the case that the solutions that we come up with in the previous steps aren't implemented in the best way. Maybe they are storing more than they need to, like we saw with our first pass at the Floyd-Warshall algorithm. In this final step (which we won't go into in too much detail in CS161), we go back through the DP solution we've designed, and optimize it for space, running time, and so on.

In this class, we'll focus mostly on 1,2, and 3. We'll see a few examples of 4, and occasionally wave our hands about 5.

2 Longest Common Subsequence

We now consider the longest common subsequence problem which has applications in spell-checking, biology (whether different DNA sequences correspond to the same protein), and more.

We say that a sequence Z is a *subsequence* of a sequence X if Z can be obtained from X by deleting symbols. For example, **abracadabra** has **baab** as a subsequence, because we can obtain **baab** by deleting **a**, **r**, **cad**, and **ra**. We say that a sequence Z is a *longest common subsequence* (LCS) of X and Y if Z is a subsequence of both X and Y , and any sequence longer than Z is not a subsequence of at least one of X or Y . For instance, the LCS of **abracadabra** and **bxqrabry** is **brabr**.

Using the definition of LCS, we define the LCS problem as follows: Given sequences X and Y , find the length of their LCS, Z (and if we are proceeding to Step 4 of the outline above, output Z).

In what follows, suppose that the sequence X is $X = x_1x_2x_3 \cdots x_m$, so that X has length m , and suppose that $Y = y_1y_2 \cdots y_n$ as length n . We'll use the notation $X[1 : k]$ as usual to denote the *prefix* $X[1 : k] = x_1x_2 \cdots x_k$.

¹We won't talk too much about this step in CS161, even though it is often important in practice.

2.1 Steps 1 and 2: Identify optimal substructure, and write a recursive formulation

Our sub-problems will be to solve LCS on prefixes of X and Y . To see how we can do this, we consider the following two cases.

- **Case 1:** $x_m = y_n$. If $x_m = y_n = \ell$, then any LCS Z has ℓ as its last symbol. Indeed, suppose that Z' is any common subsequence that does *not* end in ℓ : then we can always extend it by appending ℓ to Z' to obtain another (longer) legal common subsequence.

Thus, if $|Z| = k$ and $x_m = y_n = \ell$, we can write

$$Z[1 : k - 1] = \text{LCS}(X[1 : m - 1], Y[1 : n - 1])$$

and

$$Z = Z[1 : k - 1] \circ \ell,$$

where \circ denotes the concatenation operation on strings.

- **Case 2:** $x_m \neq y_n$. As above, let Z be the LCS of X and Y . In this case, the last letter of Z (call it z_k) is either not equal to x_m or it is not equal to y_n . (Notice that this is not an exclusive or; maybe z_k isn't equal to either x_m or y_n). In this case, at least one of x_m or y_n cannot appear in the LCS of X and Y ; this means that either

$$\text{LCS}(X, Y) = \text{LCS}(X[1 : m - 1], Y)$$

or

$$\text{LCS}(X, Y) = \text{LCS}(X, Y[1 : n - 1]),$$

whichever is longer. That is, we can shave one letter off the end of either X or Y . In particular, the length of $\text{LCS}(X, Y)$ is given by

$$\text{lenLCS}(X, Y) = \max \{ \text{lenLCS}(X[1 : m - 1], Y), \text{lenLCS}(X, Y[1 : n - 1]) \}.$$

This immediately gives us our recursive formulation. Let's keep a table C , so that

$$C[i, j] = \text{length of } \text{LCS}(X[1 : i], Y[1 : j]).$$

Then we have the relationship:

$$C[i, j] = \begin{cases} 0 & i = 0 \text{ or } j = 0 \\ C[i - 1, j - 1] + 1 & X[i] = Y[j], i, j > 0 \\ \max\{C[i - 1, j], C[i, j - 1]\} & X[i] \neq Y[j], i, j > 0 \end{cases}$$

Suppose we keep a table C , where $C[i, j]$ maintains the length of $\text{LCS}(X[1 : i], Y[1 : j])$, the longest common subsequence of $X[1 : i]$ and $Y[1 : j]$. Then, we can fill in the values of C using the following recurrence:

$$C[i, j] = \begin{cases} 1 + C[i - 1, j - 1], & \text{if } X[i] = Y[j] \\ \max(C[i - 1, j], C[i, j - 1]), & \text{otherwise} \end{cases}$$

Technically, we should do a proof here to show that this recurrence is correct. See CLRS for the details, but it is true that if we define $C[i, j]$ recursively as above, then indeed, $C[i, j]$ is equal to the length of $\text{LCS}(X[1 : i], Y[1 : j])$. (Good exercise: prove this for yourself using induction).

Algorithm 1: lenLCS(X, Y)

```
Initialize an  $n + 1 \times m + 1$  zero-indexed array  $C$ .
Set  $C[0, j] = C[i, 0] = 0$  for all  $i, j \in \{1, \dots, m\} \times \{1, \dots, n\}$ .
for  $i = 1, \dots, m$  do
    for  $j = 1, \dots, n$  do
        if  $X[i] = Y[j]$  then
             $C[i, j] \leftarrow C[i - 1, j - 1] + 1$ 
        else
             $C[i, j] \leftarrow \max\{C[i - 1, j], C[i, j - 1]\}$ 
return  $C$ 
```

2.2 Step 3: Define an algorithm using our recursive relationship.

The recursive relationship above naturally gives rise to a DP algorithm for filling out the table C :

Note that there are only $n \times m$ entries in our table C . This is where the **overlapping subproblems** come in: we only need to compute each entry once, even though we may access it many times when filling out subsequent entries.

We can also see that $C[i, j]$ only depends on three possible prior values: $C[i - 1, j]$, $C[i, j - 1]$, and $C[i - 1, j - 1]$. This means that each time we compute a new value $C[i, j]$ from previous entries, it takes time $O(1)$.

Thus, we can start to see how to obtain an algorithm for filling in the table and obtaining the LCS. First, we know that any string of length 0 will have an LCS of length 0. Thus, we can start by filling out $C[0, j] = 0$ for all j and similarly, $C[i, 0] = 0$ for all i . Then, we can fill out the rest of the table, filling the rows from bottom up (i from 1 to m) and filling each row from left to right (j from 1 to n). The pseudocode is given in Algorithm 1.

As mentioned above, in order to fill each entry, we only need to perform a constant number of lookups and additions. Thus, we need to do a constant amount of work for each of the $m \times n$ entries, giving a running time of $O(mn)$.

2.3 Step 4: Recovering the actual LCS

Algorithm 1 only computes the *length* of the LCS of X and Y . What if we want to recover the actual longest common subsequence? In Algorithm 2, we show how we can construct the actual LCS, given the dynamic programming table C that we've filled out in Algorithm 1.

In this algorithm, we start from the end of X and Y and work backward, using our table C as a guide. We start with $i = m$ and $j = n$. If at some point (i, j) , we see that $X[i] = Y[j]$, then decrement both i and j . On the other hand, if $X[i] \neq Y[j]$, then we know that we need to drop a symbol from either X or Y . The table C will tell us which: if $C[i, j] = C[i, j - 1]$, then we can drop a symbol from Y and decrement j . If $C[i, j] = C[i - 1, j]$, then we can drop a symbol from X and decrement i . Of course, it might be the case that both of these hold; in this case it doesn't matter which we decrement, and our pseudocode will be default decrement j .

How long does this take? Notice that in each step, the sum $i + j$ is decremented by at least one (maybe two) and stops as soon as one of i, j is equal to zero; this is at least before $i + j = 0$. Thus, the number of times we decrement $i + j$ is at most $m + n$, which was their total value to start.

Because at each step of Algorithm 2, the work is $O(1)$, the total running time is thus $O(n + m)$, which is subsumed by the runtime of $O(mn)$ necessary to fill in the table.

The conclusion is that we can find $\text{LCS}(X, Y)$ of a sequence X of length m and a sequence Y of length n in time $O(mn)$.

Interestingly, this simple dynamic programming algorithm is basically the best known algorithm for solving the LCS problem. It is conjectured that this algorithm may be essentially optimal. It turns out

Algorithm 2: LCS(X, Y, C)

```
// C is filled out already in Algorithm 1
 $L \leftarrow \emptyset$ 
 $i \leftarrow m$ 
 $j \leftarrow n$ 
while  $i > 0$  and  $j > 0$  do
    if  $X[i] = Y[j]$  then
        append  $X[i]$  to the beginning of  $L$ 
         $i \leftarrow i - 1$ 
         $j \leftarrow j - 1$ 
    else if  $C[i, j] = C[i, j - 1]$  then
         $j \leftarrow j - 1$ 
    else
         $i \leftarrow i - 1$ 
```

that giving an algorithm that (polynomially) improves the dependence on m and n over the $O(mn)$ strategy outlined above would imply a major breakthrough in algorithms for the boolean satisfiability problem – a problem widely believed to be computationally hard to solve.

3 The Knapsack Problem

This is a classic problem, defined as the following:

We have n items, each with a value and a positive weight. The i th item has weight w_i and value v_i . We have a knapsack that holds a maximum weight of W . Which items do we put in our knapsack to maximize the value of the items in our knapsack? For example, let's say that $W = 10$; that is, the knapsack holds a weight of at most 10. Also suppose that we have four items, with weight and value:

Item	Weight	Value
A	6	25
B	3	13
C	4	15
D	2	8

We will talk about two variations of this problem, one where you have infinite copies of each item (commonly known as Unbounded Knapsack), and one where you have only one of each item (commonly known as 0-1 Knapsack).

What are some useful subproblems? Perhaps it's having knapsacks of smaller capacities, or maybe it's having fewer items to choose from. In fact, both of these ideas for subproblems are useful. As we will see, the first idea is useful for the Unbounded Knapsack problem, and a combination of the two ideas is useful for the 0-1 Knapsack problem.

3.1 The Unbounded Knapsack Problem

In the example above, we can pick two of item B and two of item D . Then, the total weight is 10, and the total value 42.

We define $K(x)$ to be the optimal solution for a knapsack of capacity x . Suppose $K(x)$ happens to contain the i th item. Then, the remaining items in the knapsack must have a total weight of at most $x - w_i$. The remaining items in the knapsack must be an optimum solution. (If not, then we could have replaced

those items with a more highly valued set of items.) This gives us a nice subproblem structure, yielding the recurrence

$$K(x) = \max_{i: w_i \leq x} (K(x - w_i) + v_i).$$

Developing a dynamic programming algorithm around this recurrence is straightforward. We first initialize $K(0) = 0$, and then we compute $K(x)$ values from $x = 1, \dots, W$. The overall runtime is $O(nW)$.

Algorithm 3: UNBOUNDEDKNAPSACK(W, n, w, v)

```

 $K[0] \leftarrow 0$ 
for  $x = 1, \dots, W$  do
     $K[x] \leftarrow 0$ 
    for  $i = 1, \dots, n$  do
        if  $w_i \leq x$  then
             $K[x] \leftarrow \max\{K[x], K[x - w_i] + v_i\}$ 
return  $K[W]$ 

```

Remark 1. *This solution is not actually polynomial in the input size because it takes $\log(W)$ bits to represent W . We call these algorithms “pseudo-polynomial.” If we had a polynomial time algorithm for Knapsack, then a lot of other famous problems would have polynomial time algorithms. This problem is NP-hard.*

3.2 The 0-1 Knapsack Problem

Now we consider what happens when we can take at most one of each item. Going back to the initial example, we would pick item A and item C , having a total weight of 10 and a total value of 40.

The subproblems that we need must keep track of the knapsack size as well as which items are allowed to be used in the knapsack. Because we need to keep track of more information in our state, we add another parameter to the recurrence (and therefore, another dimension to the DP table). Let $K(x, j)$ be the maximum value that we can get with a knapsack of capacity x considering only items at indices from $1, \dots, j$. Consider the optimal solution for $K(x, j)$. There are two cases:

1. Item j is used in $K(x, j)$. Then, the remaining items that we choose to put in the knapsack must be the optimum solution for $K(x - w_j, j - 1)$. In this case, $K(x, j) = K(x - w_j, j - 1) + v_j$.
2. Item j is not used in $K(x, j)$. Then, $K(x, j)$ is the optimum solution for $K(x, j - 1)$. In this case, $K(x, j) = K(x, j - 1)$.

So, our recurrence relation is: $K(x, j) = \max\{K(x - w_j, j - 1) + v_j, K(x, j - 1)\}$. Now, we’re done: we simply calculate each entry up to $K(W, n)$, which gives us our final answer. Note that this also runs in $O(nW)$ time despite the additional dimension in the DP table. This is because at each entry of the DP table, we do $O(1)$ work.

4 The Independent Set Problem

This problem is as follows:

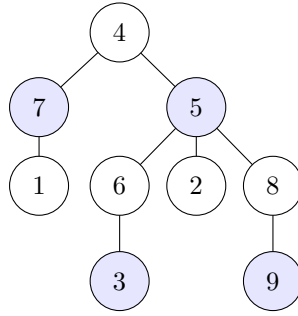
Say that we have an undirected graph $G = (V, E)$. We call a subset $S \subseteq V$ of vertices “independent” if there are no edges between vertices in S . Let vertex i have weight w_i , and denote $w(S)$ as the sum of weights of vertices in S . Given G , find an independent set of maximum weight $\operatorname{argmax}_{S \subseteq V} w(S)$.

Actually, this problem is NP-hard for a general graph G . However, if our graph is a tree, then we can solve this problem in linear time. In the following figure, the maximum weight independent set is highlighted in blue.

Remark 2. *Dynamic programming is especially useful to keep in mind when you are solving a problem that involves trees. The tree structure often lends itself to dynamic programming solutions.*

Algorithm 4: ZEROONEKNAPSACK(W, n, w, v)

```
for  $x = 1, \dots, W$  do
   $K[x, 0] \leftarrow 0$ 
for  $j = 1, \dots, n$  do
   $K[0, j] \leftarrow 0$ 
for  $j = 1, \dots, n$  do
  for  $x = 1, \dots, W$  do
     $K[x, j] \leftarrow K[x, j - 1]$ 
    if  $w_j \leq x$  then
       $K[x, j] \leftarrow \max\{K[x, j], K[x - w_j, j - 1] + v_j\}$ 
return  $K[W, n]$ 
```



As usual, the key question to ask is, “What should our subproblem(s) be?” Intuitively, if the problem has to do with trees, then subtrees often play an important role in identifying our subproblems. Let’s pick any vertex r and designate it as the root. Denoting the subtree rooted at u as T_u , we define $A(u)$ to be the weight of the maximum weight independent set in T_u . How can we express $A(u)$ recursively? Letting S_u be the maximum weight independent set of T_u , there are two cases:

1. If $u \notin S_u$, then $A(u) = \sum_v A(v)$ for all children v of u .
2. If $u \in S_u$, then $A(u) = w_u + \sum_v A(v)$ for all grandchildren v of u .

To avoid solving the subproblem for trees rooted at grandchildren, we introduce $B(u)$ as the weight of the maximum weight independent set in $T_u \setminus \{u\}$. That is, $B(u) = \sum_v A(v)$ for all children v of u . Equivalently, we have the following cases:

1. If $u \notin S_u$, then $A(u) = \sum_v A(v)$ for all children v of u .
2. If $u \in S_u$, then $A(u) = w_u + \sum_v B(v)$ for all children v of u .

So, we can calculate the weight of the maximum weight independent set:

$$A(u) = \max \left\{ \sum_{v \in \text{CHILDREN}(u)} A(v), w_u + \sum_{v \in \text{CHILDREN}(u)} B(v) \right\}$$

To create an algorithm out of this recurrence, we can compute the $A(u)$ and $B(u)$ values in a bottom-up manner (a post-order traversal on the tree), arriving at the answer, $A(r)$. This takes $O(|V|)$ time.

Algorithm 5: MAXWEIGHTINDEPENDENTSET(G) $\triangleright G$ is a tree

$r \leftarrow \text{ARBITRARYVERTEX}(G)$

$T \leftarrow \text{ROOTTREEAT}(G, r)$

Procedure SOLVESUBTREEAT(u)

if CHILDREN(T, u) = \emptyset **then**

$A(u) \leftarrow w_u$

$B(u) \leftarrow 0$

else

for $v \in \text{CHILDREN}(T, u)$ **do**

\sqsubset SOLVESUBTREEAT(v)

$A(u) \leftarrow \max \left\{ \sum_{v \in \text{CHILDREN}(T, u)} A(v), w_u + \sum_{v \in \text{CHILDREN}(T, u)} B(v) \right\}$

$B(u) \leftarrow \sum_{v \in \text{CHILDREN}(T, u)} A(v)$

SOLVESUBTREEAT(r)

return $A(r)$

1 Greedy Algorithms

Suppose we want to solve a problem, and we're able to come up with some recursive formulation of the problem that would give us a nice dynamic programming algorithm. But then, upon further inspection, we notice that any optimal solution only depends on looking up the optimal solution to one other subproblem. A greedy algorithm is an algorithm which exploits such a structure, ignoring other possible choices. Greedy algorithms can be seen as a refinement of dynamic programming; in order to prove that a greedy algorithm is correct, we must prove that to compute an entry in our table, it is sufficient to consider at most one other table entry; that is, at each point in the algorithm, we can make a "greedy", locally-optimal choice, and guarantee that a globally-optimal solution still exists. Instead of considering multiple choices to solve a subproblem, greedy algorithms only consider a single subproblem, so they run extremely quickly – generally, linear or close-to-linear in the problem size.

Unfortunately, greedy algorithms do not always give the optimal solution, but they frequently give good (approximate) solutions. To give a correct greedy algorithm one must first identify optimal substructure (as in dynamic programming), and then argue that at each step, you only need to consider one subproblem. That is, even though there may be many possible subproblems to recurse on, given our selection of subproblem, there is always an optimal solution that contains the optimal solution to the selected subproblem.

1.1 Activity Selection Problem

One problem, which has a very nice (correct) greedy algorithm, is the Activity Selection Problem. In this problem, we have a number of activities. Your goal is to choose a subset of the activities to participate in. Each activity has a start time and end time, and you can't participate in multiple activities at once. Thus, given n activities a_1, a_2, \dots, a_n where a_i has start time s_i and finish time f_i , we want to find a maximum set of non-conflicting activities.

The activity selection problem has many applications, most notably in scheduling jobs to run on a single machine.

1.1.1 Optimal Substructure

Let's start by considering a subset of the activities. In particular, we'll be interested in considering the set of activities $S_{i,j}$ that start after activity a_i finishes and end before activity a_j starts. That is, $S_{i,j} = \{a_k | f_i \leq s_k, f_k \leq s_j\}$. We can participate in these activities between a_i and a_j . Let $A_{i,j}$ be a maximum subset of non-conflicting activities from the subset $S_{i,j}$. Our first intuition would be to approach this by using dynamic programming. Suppose some $a_k \in A_{i,j}$, then we can break down the optimal subsolution $A_{i,j}$ as follows

$$|A_{i,j}| = 1 + |A_{i,k}| + |A_{k,j}|$$

where $A_{i,k}$ is the best set for $S_{i,k}$ (before a_k), and $A_{k,j}$ is the best set for after a_k . Another way of interpreting this expression is to say "once we place a_k in our optimal set, we can only consider optimal solutions to subproblems that do not conflict with a_k ."

Thus, we can immediately come up with a recurrence that allows us to come up with a dynamic programming algorithm to solve the problem.

$$|A_{i,j}| = \max_{a_k \in S_{i,j}} 1 + |A_{i,k}| + |A_{k,j}|$$

This problem requires us to fill in a table of size n^2 , so the dynamic programming algorithm will run in $\Omega(n^2)$ time. The actual runtime is $O(n^3)$ since filling in a single entry might take $O(n)$ time.

But we can do better! We will show that we only need to consider the a_k with the smallest finishing time, which immediately allows us to search for the optimal activity selection in linear time.

Claim 1. *For each $S_{i,j}$, there is an optimal solution $A_{i,j}$ containing $a_k \in S_{i,j}$ of minimum finishing time f_k .*

Note that if the claim is true, when f_k is minimum, then $A_{i,k}$ is empty, as no activities can finish before a_k ; thus, our optimal solution only depends on one other subproblem $A_{k,j}$ (giving us a linear time algorithm).

Here, we prove the claim.

Proof. Let a_k be the activity of minimum finishing time in $S_{i,j}$. Let $A_{i,j}$ be some maximum set of non-conflicting activities. Consider $A'_{i,j} = A_{i,j} \setminus \{a_l\} \cup \{a_k\}$ where a_l is the activity of minimum finishing time in $A_{i,j}$. It's clear that $|A'_{i,j}| = |A_{i,j}|$. We need to show that $A'_{i,j}$ does not have conflicting activities. We know $a_l \in A_{i,j} \subset S_{i,j}$. This implies $f_l \geq f_k$, since a_k has the minimum finishing time in $S_{i,j}$.

All $a_t \in A_{i,j} \setminus \{a_l\}$ don't conflict with a_l , which means that $s_t \geq f_l$, which means that $s_t \geq f_k$, so this means that no activity in $A_{i,j} \setminus \{a_l\}$ can conflict with a_k . Thus, $A'_{i,j}$ is an optimal solution. \square

Due to the above claim, the expression for $A_{i,j}$ from before simplifies to the following expression in terms of $a_k \subseteq S_{i,j}$, the activity with minimum finishing time f_k .

$$\begin{aligned} |A_{i,j}| &= 1 + |A_{k,j}| \\ A_{i,j} &= A_{k,j} \cup \{a_k\} \end{aligned}$$

Algorithm Greedy-AS assumes that the activities are presorted in nondecreasing order of their finishing time, so that if $i < j$, $f_i \leq f_j$.

Algorithm 1: Greedy-AS(a)

```

 $A \leftarrow \{a_1\}$  // activity of min  $f_i$ 
 $k \leftarrow 1$ 
for  $m = 2 \rightarrow n$  do
    if  $s_m \geq f_k$  then
        //  $a_m$  starts after last activity in  $A$ 
         $A \leftarrow A \cup \{a_m\}$ 
         $k \leftarrow m$ 
return  $A$ 

```

By the above claim, this algorithm will produce a legal, optimal solution via a greedy selection of activities. There may be multiple optimal solutions, but there always exists a solution that includes a_k with the minimum finishing time. The algorithm does a single pass over the activities, and thus only requires $O(n)$ time – a dramatic improvement from the trivial dynamic programming solution. If the algorithm also needed to sort the activities by f_i , then its runtime would be $O(n \log n)$ which is still better than the original dynamic programming solution.

1.2 Scheduling

Consider another problem that can be solved greedily. We are given n jobs which all need a common resource. Let w_j be the weight (or importance) and l_j be the length (time required) of job j . Our output is an ordering of jobs. We define the completion time c_j of job j to be the sum of the lengths of jobs in the ordering up to and including l_j . Our goal is to output an ordering of jobs that minimizes the weighted sum of completion times $\sum_j w_j c_j$.

1.2.1 Intuition

Our intuition tells us that if all jobs have the same length, then we prefer larger weighted jobs to appear earlier in the order. If jobs all have equal weights, then we prefer shorter length jobs in the order.

1	2	3
---	---	---

vs

3	2	1
---	---	---

In the first case, assuming they all have equal weights of 1, $\sum_{i=1}^3 w_i c_i = 1 + 3 + 6 = 10$. In the second case, $\sum_{i=1}^3 w_i c_i = 3 + 5 + 6 = 14$.

1.2.2 Optimal Substructure

What do we do in the cases where $l_i < l_j$ and $w_i < w_j$? Consider the optimal ordering of jobs. Suppose we have a job i that is followed by job j in the optimal order. Consider swapping jobs i and j . The example below swaps jobs 1 and 2.

l_1	l_2	l_2	l_1	
1	2	\rightarrow	2	1

Note that swapping jobs i and j does not alter the completion times for every other job and only changes the completion times for i and j . c_i increases by l_j and c_j decreases by l_i . This means that our objective function $\sum_i w_i c_i$ changes by $w_i l_j - w_j l_i$. Since we assumed our order was optimal originally, our objective function cannot decrease after swapping the jobs. This means,

$$w_i l_j - w_j l_i \geq 0$$

which implies,

$$\frac{l_j}{w_j} \geq \frac{l_i}{w_i}$$

Therefore, we want to process jobs in increasing order of $\frac{l_i}{w_i}$, the ratio of the length to the weight of each job. The algorithm also does a single pass over jobs, and thus only requires $O(n)$ time, assuming the jobs were ordered by $\frac{l_i}{w_i}$. Like previously, if the algorithm also needed to sort the jobs based on the ratio of length to weight, then its runtime would be $O(n \log n)$.

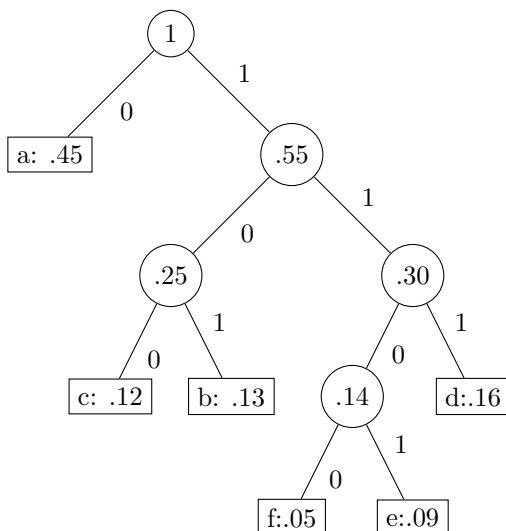
1.3 Optimal Codes

Our third example comes from the field of information theory. In ASCII, there is a fixed 8 bit code for each character. Suppose we want to incorporate information about frequencies of characters to obtain shorter encodings. What if we want to represent characters by codes of different lengths depending on each character's frequencies? We explore a greedy solution to find the optimal encoding of characters.

To create optimal codes, we want a way to encode and decode our sequence. To encode the sequence, we would just have to concatenate the code of each character together. How about for decoding? Consider the following codes of characters: $a \rightarrow 0, b \rightarrow 1, c \rightarrow 01$. However, when decoding, when we encounter 01, this could be decoded as "ab" or "c". Therefore, our codes need to be **prefix free**: no codeword is a prefix of another.

1.3.1 Tree Representation

We may think of representing our codes in a tree structure, where the codewords represent the leaves of our tree. An example is shown below:



Above, in addition to the characters $\{a, b, c, d, e, f\}$, we've included *frequency information*. That is, $f(a) = 0.45$ means that the probability of a random character in this language being equal to a is .45.

The code for each character can be found by concatenating the bits of the path from the root to the leaves. By convention, every left branch is given the bit 0 and every right branch is given the bit 1.

As long as the characters are on the leaves of this tree, the corresponding code will be prefix-free. This is because one string is a prefix of another if and only if the node corresponding to the first is an ancestor of the node corresponding to the second. No leaf is an ancestor of any other leaf, so the code is prefix-free.

1.3.2 How good is a code?

Suppose we have a set of characters C with frequencies $f(c)$ so that $\sum_{c \in C} f(c) = 1$. That is, $f(c)$ can be thought of as the probability of using a letter c in this language. The *cost*, in terms of bits, of a character $c \in C$ when using the coding scheme represented by a tree T is just the depth in the tree T : $\text{cost}(c) = d_T(c)$. For example, in the tree above, e has depth 4 in the tree, and requires 4 bits to represent. The average cost of the tree is

$$B(T) = \mathbb{E}_{c \in C} d_T(c) = \sum_{c \in C} f(c) d_T(c).$$

We say that a tree T is *optimal* if this expected cost $B(T)$ is as small as possible.

1.3.3 Huffman Codes

In 1951, David A. Huffman, in his MIT information theory class, was given the choice of a term paper or final exam. Huffman chose to do the term paper rather than take the final exam. He found greedy algorithm to find the most efficient binary code, which we know today as **Huffman codes**.

The basic idea is this: build subtrees for subsets of characters and merge them from the bottom up, combining the two trees with the characters of minimum total frequency.

Input: Set of characters $C = \{c_1, c_2, \dots, c_n\}$ of size n , and $F = \{f(c_1), f(c_2), \dots, f(c_n)\}$, a set of frequencies.

- Create nodes N_k for each character c_k , with key $f(c_k)$.
- Let **current** denote the set $\{N_1, \dots, N_n\}$ of nodes.
- while **current** has length more than one:
 - Find the two nodes N_i and N_j in **current** with the minimum frequencies and create a new intermediate node I with N_i and N_j as its children, so that $I.key = N_i.key + N_j.key$.
 - Add I to **current** and remove N_i, N_j .
- Return the only entry of **current**, which is the root of the tree.

Figure 1: A high-level version of the HUFFMAN CODING algorithm.

The tree shown above results from running this algorithm on the letters with those frequencies; see the slides for an illustration of this process.

1.3.4 Proof of Correctness

This algorithm works, but at first it's not at all obvious why. For a rigorous proof, refer to Lemmas 16.2 and 16.3 in CLRS. However, we'll sketch the idea below. Formally, the proof goes by induction. Recall that after iteration t in Algorithm 1, we have a list **current**, which contains the roots of subtrees that we still need to merge up. We will maintain the following inductive hypothesis:

- **Inductive Hypothesis:** Suppose we have completed t iterations of the loop in Algorithm 1. Then there exists a way to merge the subtrees in **current** that is optimal.
- For the **base case**, we observe that when $t = 0$, **current** is just the set of all characters, and definitionally there exists an optimal tree made out of these nodes.
- For the **inductive step**, we need to show that if the inductive hypothesis holds at step $t - 1$, then it holds at step t . We'll sketch this later.
- Finally, to **conclude** the argument, we see that at the end of the algorithm, there is only one element in **current**, and in this case the inductive hypothesis reads that there is a way to merge this single subtree to obtain an optimal subtree. That's just a convoluted way of saying that the single tree we return is optimal, and so we are done.

All that remains to show is the inductive step. We first observe the following claim:

Claim 2. *We are given a set of characters C and a set of its associated frequencies F where $f(c)$ is the frequency of character c . Let x and y be the characters with the two smallest frequencies. There exists an optimal coding tree for C such that x, y are sibling leaves.*

Proof. Let T be the optimal coding tree for C . The optimal coding tree must be a full binary tree, that is, every non-leaf node must have two children. Let a, b be characters that are sibling leaves of maximum depth. We define the number of bits to encode c as $d_T(c)$ and the number of bits needed for the coding tree as $B(T) = \sum_c f(c)d_T(c)$.

We can replace a, b by x, y without increasing the total number of bits needed for the coding tree.¹ If we swap x and a , the change in cost becomes

$$f(x)d_T(a) + f(a)d_T(x) - f(x)d_T(x) - f(a)d_T(a) = (f(x) - f(a))(d_T(a) - d_T(x)) \leq 0$$

¹For simplicity, we ignore the case where a, b, x, y are not distinct. For more details, see Lemma 16.2 in CLRS.

Therefore, there swapping a, b with x, y will not increase our objective function $B(T)$. Hence, there exists an optimal coding tree where x, y are siblings in the tree. \square

Claim 2 shows that there exists an optimal coding tree where x and y are sibling leaves, that is, there is an optimal code that makes the same greedy choice as the algorithm. However, this is only immediately helpful for the first iteration of the inductive step, when all of the elements of **current** are indeed leaves. In order to make this idea work for all t , we need one more claim.

Claim 3. *Let C be a set of characters, and let T be a coding tree for C . Imagine creating C' from C by collapsing all the characters in a subtree rooted at a node N with key $k = N.\text{key}$ into a single character c' with frequency k . Then the corresponding tree T' is optimal for C' .*

Conversely, suppose that a tree T' that is an optimal coding tree for an alphabet C' . Let $c' \in C'$ be a character with frequency $f(c')$. Introduce new characters c''_1, \dots, c''_r with total frequency $\sum_{i=1}^r f(c''_i) = f(c')$. Let T'' be an optimal coding tree on c''_1, \dots, c''_r . Then the tree T on the alphabet $C = (C' \setminus \{c'\}) \cup \{c''_1, \dots, c''_r\}$ that has the leaf c' replaced with the subtree T'' is optimal.

Proof. Let T and T' be the two trees described in the lemma, and consider the difference of their costs.

$$\begin{aligned}
B(T) - B(T') &= \sum_{c \in C} f(c) \cdot d_T(c) - \sum_{c \in C'} f(c) \cdot d_{T'}(c) \\
&= \left(\sum_{i=1}^r f(c''_i) d_T(c''_i) \right) - f(c') d_{T'}(c') \\
&= \left(\sum_{i=1}^r f(c''_i) (d_{T''}(c''_i) + d_{T'}(c')) \right) - f(c') d_{T'}(c') \\
&= \sum_{i=1}^r f(c''_i) d_{T''}(c''_i) + d_{T'}(c') \sum_{i=1}^r f(c''_i) - f(c') d_{T'}(c') \\
&= \sum_{i=1}^t f(c''_i) d_{T''}(c''_i)
\end{aligned}$$

where the last line used the fact that $\sum_{i=1}^r f(c''_i) = f(c')$, and so the last two terms cancelled. This means that the difference in the cost between these two trees *only* depends on T'' , it doesn't depend at all about the structure of T . Thus, T is optimal if and only if T' is optimal. \square

The two Claims together prove the inductive step, because the second claim implies that the logic of the first claim holds, even for newly created intermediate nodes I .

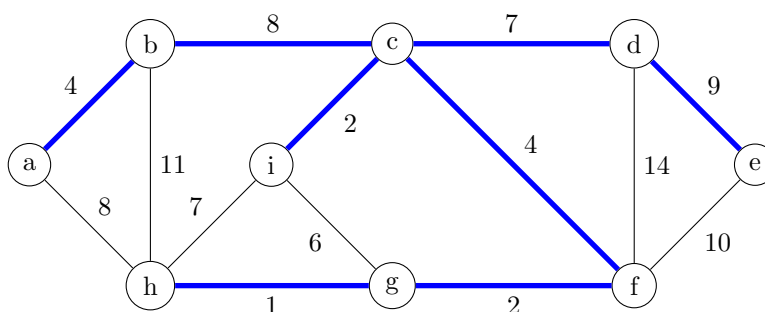
Note: The proof in CLRS has the same basic steps (Lemmas 16.2 and 16.3 instead of the claims above), although phrased slightly differently. The sketch above is pretty sketchy, so if the above is hard to follow, please check out CLRS for a more detailed version.

1 Introduction

Today we will continue our discussion of greedy algorithms, specifically in the context of computing minimum spanning trees. There are many useful applications for finding a minimum spanning tree of a graph from efficient network design to graph clustering analysis and much more. We will also show that we can compute a minimum spanning tree of a graph in polynomial time using some intuitive greedy algorithms.

The minimum spanning tree problem is formulated informally as follows: we are provided an undirected graph $G = (V, E)$ with weights $w(e) \in \mathbb{R}$ for $e \in E$ and we want to compute a subgraph of G that is a tree which connects all vertices in V (a spanning tree) and has minimum total edge weight defined as $w(T) = \sum_{e \in T} w(e)$.

Below is an example of an MST of a graph. In the example, the edges forming the MST are colored blue while edges that are not part of the MST are colored black:



2 A Template for Minimum Spanning Tree Algorithms

Let's start by introducing a basic algorithm template which will guide our discussion towards the actual algorithms for computing MSTs. These algorithms will in general follow the steps described in the template below:

Algorithm 1: Template for Minimum Spanning Tree Algorithms

```

 $A \leftarrow \emptyset$ 
while  $A$  is not a spanning tree do
  find edge  $(u, v)$  that is 'safe' for  $A$ 
   $A \leftarrow A \cup \{u, v\}$ 
return  $A$ 

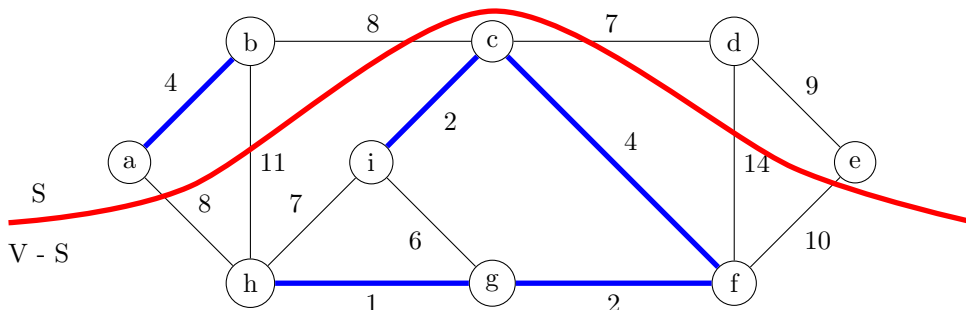
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We will show that the template results in a valid MST by maintaining the invariant that there exists at least one MST which contains all the edges in A . An edge is considered safe to add to A as long as it maintains this invariant. We will see that this definition of a safe edge can informally be defined as the edge with minimum weight which would not form a cycle if included in A . The next section will introduce new terminology to define this formally.

¹Some of the figures in these notes are taken from CLRS.

3 Cuts and Light Edges

We will introduce the notion of graph cuts to formally discuss which edges can be considered safe to add to the MST edge set. Let a *cut* $(S, V - S)$ of a graph $G = (V, E)$ be a partition of V into two disjoint sets S and $V - S$. From this, we can say that an edge (u, v) *crosses* the cut $(S, V - S)$ if the edge has one endpoint in S and the other in $V - S$. We can also say that a cut *respects* a subset A of edges if no edges in A cross the cut. An edge is considered a *light edge* crossing a cut if its weight is the minimum of any edge crossing the cut.

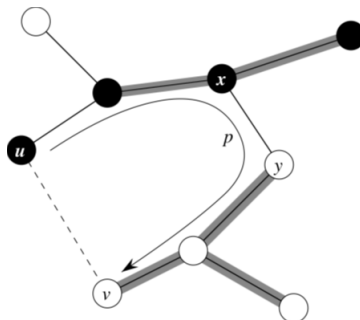


In the example above, let $(S, V - S)$ be a cut of the graph where S contains the set of nodes above the red curve and $V - S$ contains the set of nodes below it, and the set A be the set of edges colored blue. The edges which cross the cut are exactly the following: (a, h) , (b, h) , (b, c) , (c, d) , (d, f) , (e, f) and the only light edge which crosses $(S, V - S)$ is (c, d) . Since none of these edges are contained in the set A , the cut respects the set A . Note that if we were to add any of the edges previously mentioned to A , then the cut would no longer respect A .

Given the definitions above, let $G = (V, E)$ be a connected and undirected graph with edge weights $w(e)$, A be a subset of E such that some MST of G contains A , $(S, V - S)$ be a cut that respects A , and (u, v) be a light edge crossing $(S, V - S)$.

Theorem 3.1. *There exists an MST that contains $A \cup \{(u, v)\}$.*

Proof. Let T be an MST containing A . As previously mentioned, (u, v) is a light edge which crosses the cut $(S, V - S)$. Since T is already a spanning tree, note that adding any other edge of the graph to it will lead to a cycle, so in particular adding (u, v) to T produces a cycle. Consider a path p from u to v in T . There will necessarily be at least one edge (x, y) of p which crosses the cut $(S, V - S)$ where $(x, y) \notin A$ because the cut respects A . Since (u, v) is a light edge, $w(u, v) \leq w(x, y)$. Deleting (x, y) from T and adding (u, v) yields a new MST T' . The only difference between T and T' are the edges (x, y) and (u, v) so $w(T') \leq w(T)$. T' is an MST which contains $A \cup \{(u, v)\}$. \square



Note that in the proof, if $w(T') \neq w(T)$, then we have that our initial assumption of T being an MST is false since we have found a spanning tree with smaller total edge weight.

Because of the theorem, we can add some additional points about the MST algorithm template.

- The MST algorithm maintains a subset A of edges with no cycles. That is, the graph represented by $G_A = (V, A)$ is a forest (a set of distinct unconnected trees).
- Any safe edge (u, v) connects two distinct connected components of G_A .
- For some connected component $C = (V_C, E_C)$ in G_A , the safe edge (u, v) is a light edge crossing $(V_C, V - V_C)$.

4 Prim's Algorithm

At a high level, the set A maintained by Prim's algorithm is a single tree. The algorithm starts with an arbitrary root r and in each step, a light edge leading out of A and connecting to a node that has not yet been connected to A is selected and added to A . Once A connects every node in the graph, it is returned as an MST of the graph.

Prim's algorithm is similar to Dijkstra's algorithm in that estimates of the distance to each node are maintained and updated as the algorithm progresses. Q is a priority queue maintaining distances of vertices not in the tree so far, $\text{key}(v)$ is the minimum weight of edge connecting v to some vertex in the tree, and $p(v)$ is the parent of v in the tree.

Algorithm 2: Prim(G)

```

key( $v$ )  $\leftarrow \infty$ ,  $\forall v \in V$ 
key( $r$ )  $\leftarrow 0$ 
 $Q \leftarrow (\text{key}(v), v)$ ,  $\forall v \in V$ 
 $p(v) \leftarrow \text{NIL}$ ,  $\forall v \in V$ 
 $A \leftarrow \emptyset$ 
while  $Q$  is not empty do
     $u \leftarrow \text{ExtractMin}(Q)$ 
    if  $u \neq r$  then
         $A = A \cup \{(p(u), u)\}$ 
        for each neighbor  $v$  of  $u$  do
            if  $v \in Q$  and  $w(u, v) < \text{key}(v)$  then
                key( $v$ ) =  $w(u, v)$ 
                DecreaseKey(key( $v$ ),  $v$ )
                 $p(v) = u$ 
return  $A$ 

```

Correctness Much of the correctness of Prim's algorithm follows from Theorem 3.1. Notice that at the beginning of every loop iteration, $A = \{ (p(v), v) : v \in (V - \{r\} - Q) \}$ meaning that the vertices already placed in the partial MST are those in $V - Q$. For all vertices $v \in Q$, if $p(v) \neq \text{NIL}$, then $\text{key}(v)$ is the minimum weight of an edge connecting v to the partial MST. This can be thought of in terms of graph cuts with partitions $(Q, V - Q)$ and the vertices in Q with non-NIL parents as being the tail of edges crossing this cut. Since in Q , only the vertices with non-NIL parents have $\text{key} \neq \infty$ (except for r in the first iteration), this means that only the edges which cross the cut are considered at each iteration and the one with minimum weight is added to A . This is exactly what the MST template algorithm does (we add a safe edge) and as such, the correctness of the algorithm follows.

Running time Prim's Algorithm can be implemented as a direct modification of Dijkstra's Algorithm and can achieve a similar running time, but its exact bound depends on the implementation of the priority queue.

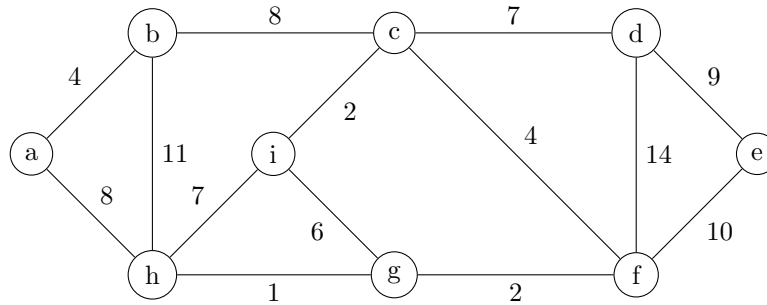
If a red-black tree or a binary heap is used:

- ExtractMin: $O(\log n)$
- DecreaseKey: $O(\log n)$
- Total: $O(n \log n + m \log n) = O(m \log n)$

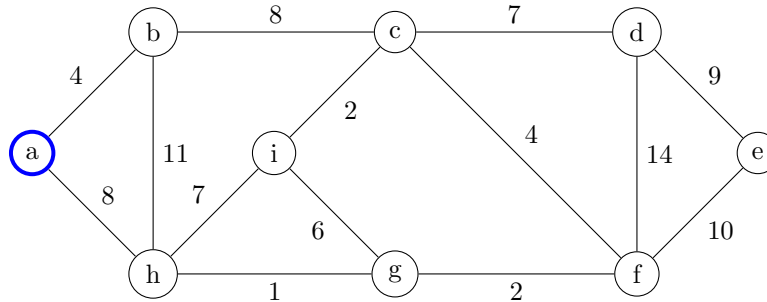
If a Fibonacci heap is used:

- ExtractMin: $O(\log n)$
- DecreaseKey: $O(1)$ amortized
- Total: $O(n \log n + m)$

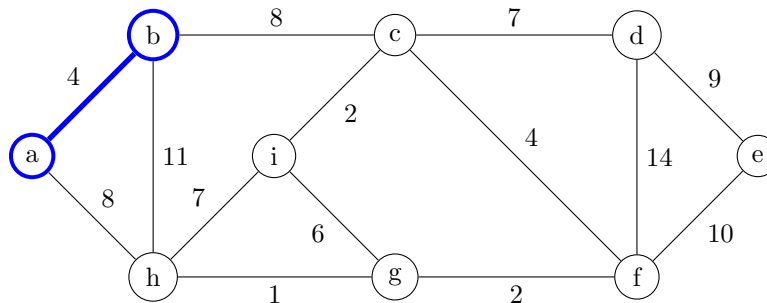
Example In this example we will run through the steps of Prim's algorithm in order to find an MST for the following graph:



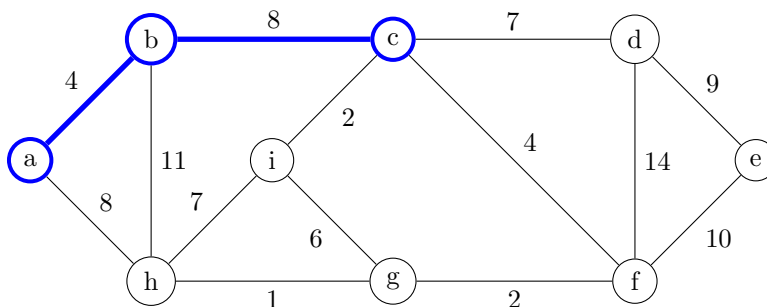
Suppose we select node a to be the source node, r . We then extract node a from Q and set $\text{key}(b) = 4$, $p(b) = a$, $\text{key}(h) = 8$, and $p(h) = a$.



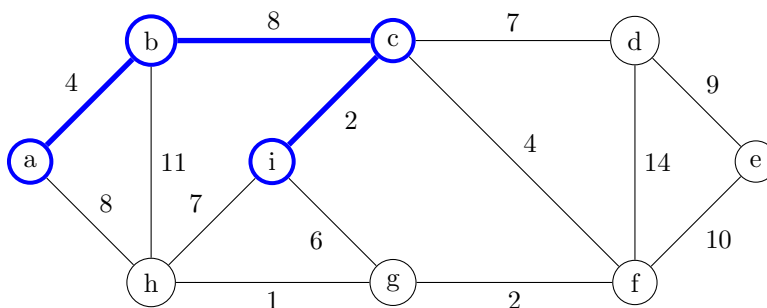
Since $\text{key}(b)$ is now the smallest value in the priority queue, we visit node b . Because $p(b) = a$ we add edge (a, b) to the set A . We then update the keys and parent fields of nodes that have edges connecting to b . Thus we set $\text{key}(c) = 8$ and $p(c) = b$.



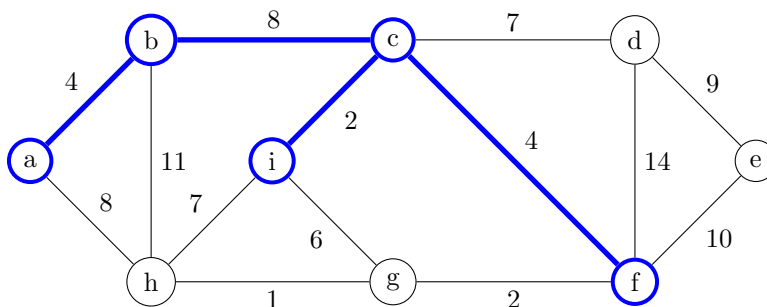
The next smallest in the priority queue is a tie between $\text{key}(c)$ and $\text{key}(h)$. The algorithm can pick either one – the results may be different, but both will be an MST. Let's say the algorithm arbitrarily picks c . We add edge (b, c) to A and perform the following updates: $\text{key}(d) = 7$, $p(d) = c$, $\text{key}(f) = 4$, $p(f) = c$, $\text{key}(i) = 2$, and $p(i) = c$.



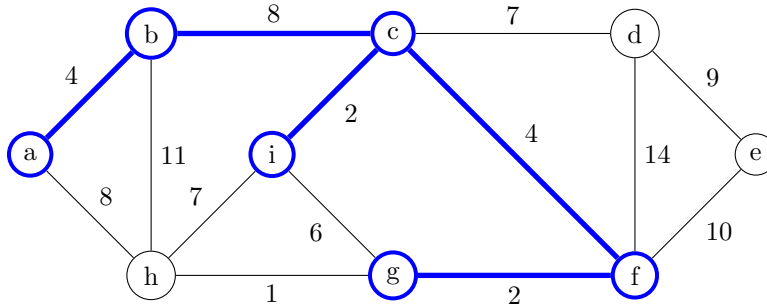
$\text{key}(i)$ is the smallest so we visit node i . Update the following: $\text{key}(g) = 6$, $p(g) = i$, $\text{key}(h) = 7$, and $p(h) = i$.



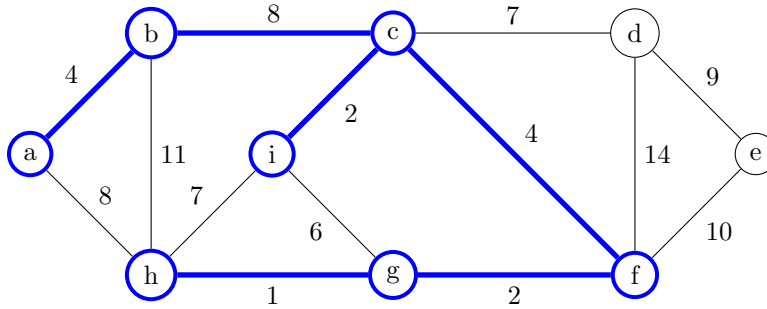
$\text{key}(f)$ is the smallest so we visit node f . Update the following: $\text{key}(g) = 2$, $p(g) = f$, $\text{key}(e) = 10$, and $p(e) = f$.



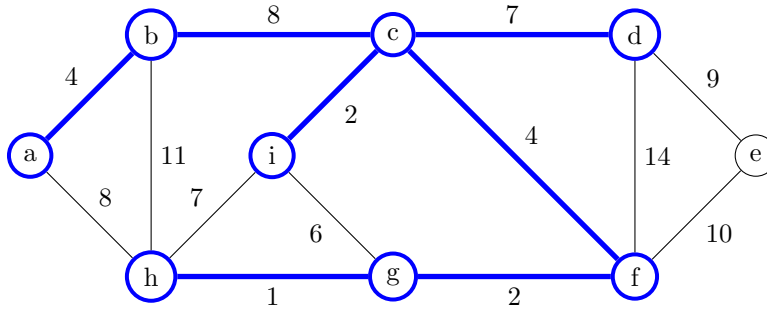
$\text{key}(g)$ is the smallest so we visit node g . Update the following: $\text{key}(h) = 1$ and $p(h) = g$.



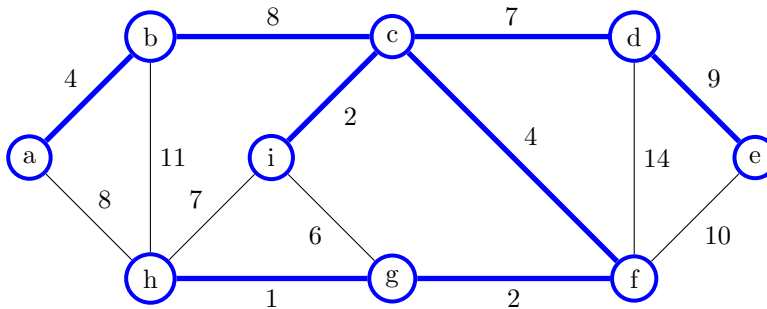
$\text{key}(h)$ is the smallest so we visit node h . There are no updates at this step.



$\text{key}(d)$ is the smallest so we visit node d . Update the following: $\text{key}(e) = 9$ and $p(e) = d$.



Finally, $\text{key}(e)$ is the smallest so we visit node e . There are no updates at this step and the algorithm will detect that Q is empty at the next iteration and return.



5 Kruskal's Algorithm

At a high level, the set A maintained by Kruskal's algorithm is a set of disjoint trees. During update step i , if the i th smallest edge connects different trees, merge the two trees connected by this edge. The algorithm progresses until eventually only one tree remains at which point the set A represents an MST of the graph.

Kruskal's algorithm utilizes the union-find (aka disjoint set) data structure in order to handle the merging of the disjoint trees maintained by the algorithm. The union-find data structure supports disjoint sets with the following operations:

- **makeset**(u): creates a new set containing u provided that u is not in any other set
- **find**(u): returns the name of the set containing u
- **union**(u, v): merge the set containing u and the set containing v into one set

The algorithm itself can be structured as follows:

Algorithm 3: Kruskal(G)

```

 $A \leftarrow \emptyset$ 
 $E' \leftarrow$  sort edges by weight in non-decreasing order
foreach  $v \in V$  do
     $\mid$  makeset( $v$ )
foreach  $(u, v) \in E'$  do
     $\mid$  if find( $u$ )  $\neq$  find( $v$ ) then
     $\mid \mid$   $A \leftarrow A \cup \{(u, v)\}$ 
     $\mid \mid$  union( $u, v$ )
return  $A$ 

```

Correctness The correctness follows from Theorem 3.1.

Running time The runtime of Kruskal's algorithm depends on two factors: the time to sort the edges by weight and the runtime of the union-find data structure operations. While $\Omega(m \log n)$ time is required for sorting the edges if we use comparison-based sorting, in many cases, we may be able to sort the edges in linear time. (Recall, that RadixSort can be used to sort the edges in $O(m)$ time if the weights are given by integers bounded by a polynomial in m .) In this case, the runtime is bounded by the runtime of the union-find operations and is given by $O(nT(\text{makeset}) + mT(\text{find}) + nT(\text{union}))$. The best known data structure supporting the union-find operations runs in amortized time $O(\alpha(n))$ where $\alpha(n)$ is the inverse Ackermann function. Interestingly, the value of the inverse Ackermann is tiny for all practical purposes:

$$\alpha(n) \leq 4, \quad \forall n < \# \text{ atoms in the universe}$$

and thus for all practical purposes, the union-find operations run in constant time. Thus, in many settings, the runtime of Kruskal's algorithm is nearly linear in the number of edges.

The actual definition of $\alpha(n)$ is $\alpha(n) = \min\{k \mid A(k) \geq n\}$, where $A(k)$ is the Ackermann function evaluated at k . $A(k)$ itself is defined using the more general Ackermann function as $A(k) = A_k(2)$. $A_k(x)$ is defined recursively:

$$A_m(x) = \begin{cases} x + 1 & m = 0 \\ A_{m-1}(1) & m > 0, x = 0 \\ A_{m-1}(A_m(x - 1)) & \text{else} \end{cases}$$

For example

- $A_0(x) = 1 + x$, so $A_0(2) = 3$.
- To compute $A_1(x)$, we see:

$$A_1(x) = A_0(A_1(x-1)) = A_0(A_0(A_1(x-2))) = \cdots = A_0(A_0(\cdots(A_0(A_1(0))))) = A_0(A_0(\cdots(A_0(2)))),$$

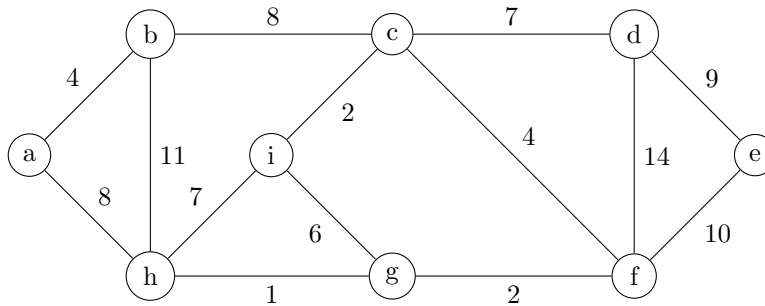
that is, we have “iterated” A_0 x times. If we work it out, we get

$$A_1(x) = 2x.$$

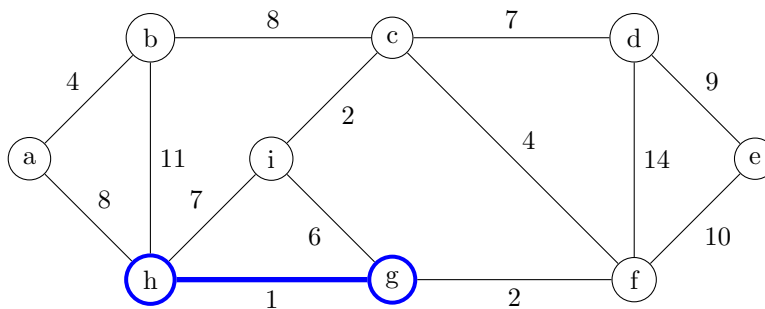
Thus, $A_1(2) = 4$.

- $A_2(x) = 2^x x$ (A_1 iterated x times), so $A_2(2) = 8$
- $A_3(x) \geq 2^{2^{2^{\cdots}}}$, a “tower” of x 2s (A_2 iterated x times); it turns out $A_3(2) \geq 2^{11}$
- $A_4(x)$ is larger than the total number of atoms in the known universe, and also larger than the number of nanoseconds since the Big Bang. (Thus, $\alpha(n) \leq 4$ for all practical purposes.)

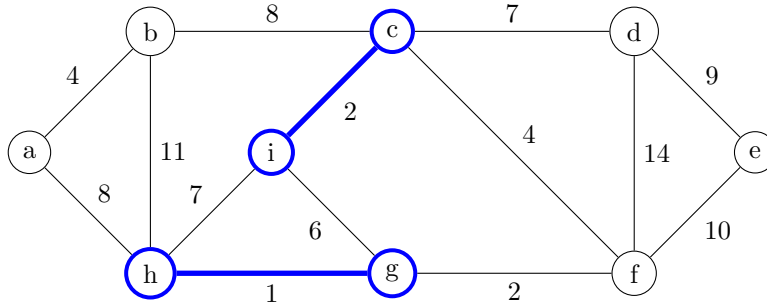
Example In this example we will run through the steps of Kruskal’s algorithm in order to find an MST for the following graph:



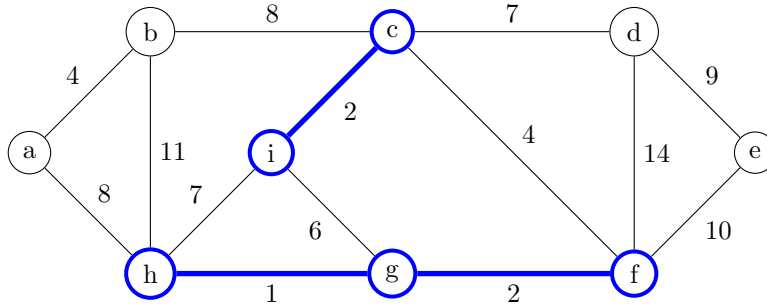
We begin by creating a new set for each node in the graph. We then begin iterating over the edges in non-decreasing order. The first edge we examine is (g, h) . This edge connects nodes g and h which are currently not part of the same set. We thus include this edge in A and union the sets containing g and h .



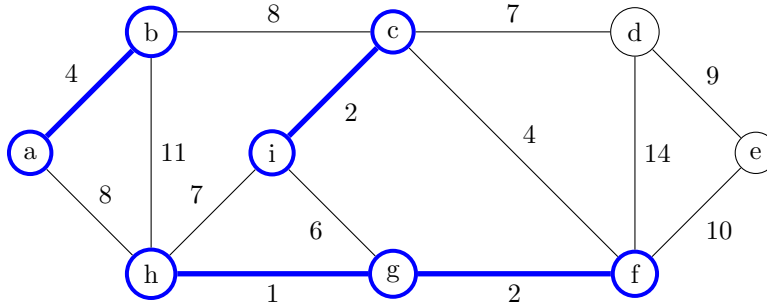
The next edge in the sorted order is a tie between edges (c, i) and (f, g) . Picking either one will yield a correct result, so let’s say the algorithm picks (c, i) . Since c and i are not part of the same set we include this edge in A and union the sets containing c and i .



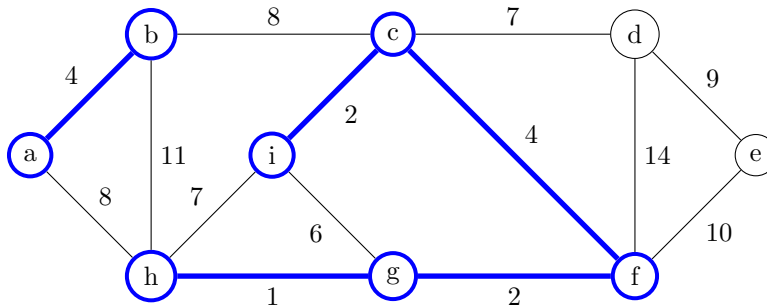
The next edge in the sorted order is (f, g) . We union the sets containing f and g and add edge (f, g) to A .



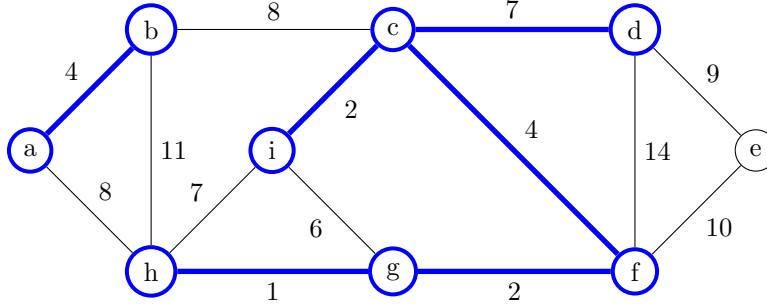
The next edge in the sorted order is a tie between edges (a, b) and (c, f) . Let's say the algorithm picks (a, b) . We union the sets containing a and b and add edge (a, b) to A .



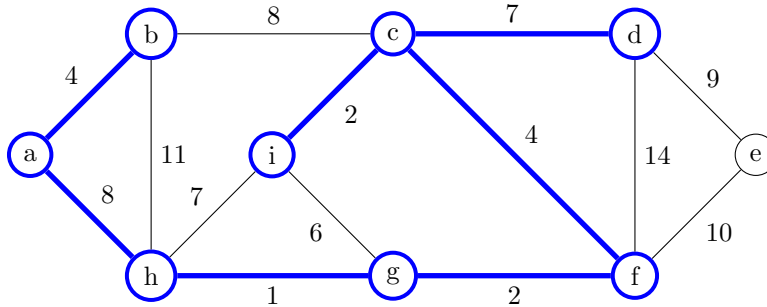
The next edge in the sorted order is (c, f) . We union the sets containing c and f and add edge (c, f) to A .



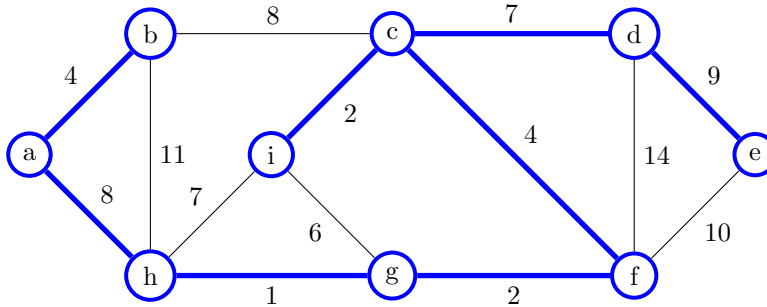
The next edge in the sorted order is (i, g) . Note that i and g are contained in the same set which means that adding the edge (i, g) would lead to a cycle in A . We therefore ignore (i, g) and pick the next edge in sorted order which is a tie between (c, d) and (h, i) . Let's say the algorithm picks (c, d) . We union the sets containing c and d and add edge (c, d) to A .



The next edge in the sorted order is (h, i) , but h and i are contained in the same set so we ignore it. The next edge is a tie between edges (a, h) and (b, c) . Let's say the algorithm picks (a, h) . We union the sets containing a and h and add edge (a, h) to A .



The next edge in the sorted order which has both vertices in different sets is (d, e) . We union the sets containing d and e and add edge (d, e) to A . At this point all nodes are contained in the same set, so no further edges are added to A .



6 The Latest and Greatest Algorithms

While the greedy algorithms mentioned above are reasonably efficient ways to compute a minimum spanning tree of a graph, recent research has yielded more efficient algorithms. In 1995, Karger, Klein, and Tarjan discovered a randomized linear time ($O(E + V)$) algorithm based on Borůvka's algorithm and the reverse-delete algorithm. In 2000, Chazelle discovered the current fastest deterministic algorithm which runs in time $O(E\alpha(V))$ using soft heaps where α is the inverse Ackermann function.

1 History of Flows and Cuts

Today we will continue the theme of studying cuts in graphs. In particular we will be studying a very interesting problem called the max flow problem. Before that, a short history lesson. During the Cold War, the US Air Force at that time was very interested in the Soviet train networks. In reports that were declassified in 1999, it was revealed that the Air Force collected enough information about the train network that they were able to determine how resources were shipped from the Soviet Union to Europe. The Air Force was very interested in determining how much resources can be transported from the Soviet Union to Europe, and what needed to be done to destroy this movement of resources. What this translates to is the min cut problem, i.e., cut the minimum number of train tracks so that nothing goes to Europe. Here, cutting an edge means dropping a bomb. Nowadays, however, there are much milder (but still important!) applications of this problem, for instance, understanding the flow of information through the Internet.

2 Formulation of the Maximum Flow Problem

You are given an input graph $G = (V, E)$, where the edges are directed. There is a function $c : E \rightarrow \mathbb{R}^+$ that defines the capacity of each edge. We also label two nodes, s and t in G , as the source and destination, respectively. The task is to output a *flow of maximum value*. We will shortly define what a *flow* is and what a flow of *maximum value* means.

A flow f is a function $f : E \rightarrow \mathbb{R}_0^+$ such that

1. (Capacity Constraint)

$$\forall (u, v) \in E, 0 \leq f(u, v) \leq c(u, v)$$

2. (Flow Conservation Constraint)

$$\forall v \in V \setminus \{s, t\}, \sum_{x \in N_{in}(v)} f(x, v) = \sum_{y \in N_{out}(v)} f(v, y)$$

Here $N_{in}(v)$ denotes the set of nodes with an edge that points to v and $N_{out}(v)$ denotes the set of nodes that v points to.

Suppose that there are no edges going into s and no edges coming out of t . From the above, you can verify yourself that $\sum_{x \in N_{out}(s)} f(s, x) = \sum_{y \in N_{in}(t)} f(y, t)$. We define the value $\sum_{x \in N_{out}(s)} f(s, x)$ to be the value of the flow f . We usually denote the value of a flow f as $|f|$. If there are edges going into s and out of t , then the value of f is

$$|f| = \sum_{x \in N_{out}(s)} f(s, x) - \sum_{y \in N_{in}(s)} f(y, s).$$

The max flow problem is to find some flow f such that $|f|$ is maximized.

Remark 1. In the analysis below we consider graphs with a single source s and a single sink t . However, if we need to work with a graph with multiple sources, we can do so by adding a new source node, and then adding edges with capacity infinity from it to each of the multiple sources. Similarly, if we want to have multiple sinks, we add a new sink node and add edges from the multiple sinks to that sink with capacity infinity.

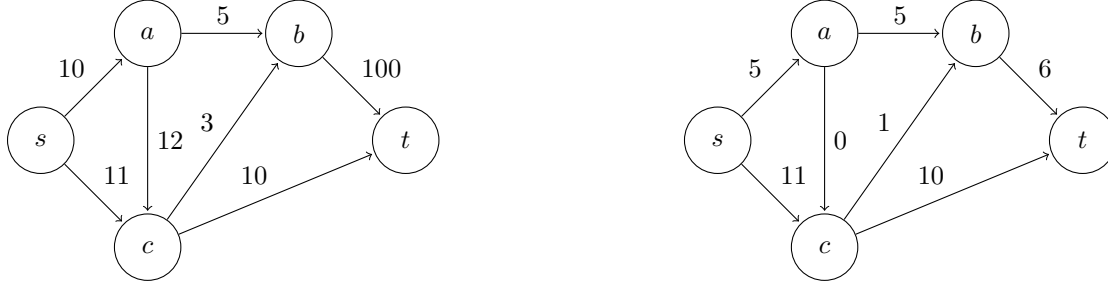


Figure 1: (Left) Graph G with edge capacities (Right) Graph G with a sample flow

3 Example

In Figure 1, we have a graph G and a sample flow f . Observe that the two constraints for a flow are satisfied. There can be multiple other flows possible that can satisfy the constraints. For our given flow, $|f| = 16$. The max flow for this graph is actually 18, as we will see shortly.

4 Formulation of the Minimum Cut Problem

Now, we give a formulation of the min cut problem defined for directed graphs with source and destination nodes s and t . (There is also a version of the Min-Cut problem without a source and sink node, though we won't discuss that now.)

An $s - t$ cut is a partition $V = S \cup T$ where S and T are disjoint and $s \in S, t \in T$, and the size/cost of an $s - t$ cut is

$$\|S, T\| = \sum_{x \in S, y \in T} c(x, y)$$

For our graph G shown above, if we set $S = \{s, a, c\}$ and $T = \{b, t\}$, then the cost of the cut is $c(a, b) + c(c, b) + c(c, t) = 5 + 3 + 10 = 18$. If we take another cut $S' = \{s, c\}, T' = \{a, b, t\}$, then $\|S', T'\| = c(s, a) + c(c, b) + c(c, t) = 10 + 3 + 10 = 23$. Note that we **do not** consider the edge $\{a, c\}$ as it is in the wrong direction (we only consider edges from S' to T').

5 The Max-Flow Min-Cut Theorem

Lemma 5.1. For any flow f and any $s - t$ cut (S, T) of G , we have $|f| \leq \|S, T\|$. In particular, the value of the max flow is at most the value of the min cut.

Proof.

$$\begin{aligned} |f| &= \sum_{x \in N_{out}(s)} f(s, x) - \sum_{y \in N_{in}(s)} f(y, s) \\ &= \sum_{v \in S} \left(\sum_{x \in N_{out}(v)} f(v, x) - \sum_{y \in N_{in}(v)} f(y, v) \right) \quad [\text{by the Flow Conservation Constraint all added terms sum to 0}] \\ &= \sum_{v \in S} \left(\sum_{x \in N_{out}(v) \cap T} f(v, x) - \sum_{y \in N_{in}(v) \cap S} f(y, v) \right) + \sum_{v \in S} \left(\sum_{x \in N_{out}(v) \cap T} f(v, x) - \sum_{y \in N_{in}(v) \cap T} f(y, v) \right) \end{aligned}$$

$$\begin{aligned}
&= \sum_{v \in S} \left(\sum_{x \in N_{out}(v) \cap T} f(v, x) - \sum_{y \in N_{in}(v) \cap T} f(y, v) \right) \quad [\text{first term sums to 0}] \\
&\leq \sum_{v \in S, x \in T, x \in N_{out}(v)} f(v, x) \leq \sum_{v \in S, x \in T, x \in N_{out}(v)} c(v, x) = \|S, T\|
\end{aligned}$$

In the proof, $\sum_{v \in S} \left(\sum_{x \in N_{out}(v) \cap S} f(v, x) - \sum_{y \in N_{in}(v) \cap S} f(y, v) \right) = 0$ since we add and subtract the flow $f(u, v)$ for every $u, v \in S$ such that $(u, v) \in E$. \square

We get the following consequence.

Corollary 5.1. If we can find f and (S, T) such that $|f| = \|S, T\|$, then f is a max flow and (S, T) is a min cut.

It turns out that we can always find such f and (S, T) for any graph.

Theorem 5.1 (Max-flow min-cut theorem). For any graph G , source s and destination t , the value of the max flow is equal to the cost of the min cut.

We will show this by coming up with an algorithm. The algorithm will take the graph G and some flow f that has already been constructed, and create a new graph that is called the residual graph. In this new graph, the algorithm will try to find a path from s to t . If no such path exists, we will show that the value of the flow we started with is the value of the maximum flow. If not, we show how to increase the value of our flow by pushing some flow on that path.

6 The Ford-Fulkerson Max-Flow Algorithm

We will make an assumption on our graph. The assumption can be removed, but it will make our lives easier. We will assume that for all $u, v \in V$, G does not have both edges (u, v) and (v, u) in E . We can make this condition hold by modifying the original graph in the following way. If $(u, v), (v, u) \in E$, we split the edge (u, v) to two edges (u, x) and (x, v) , where x is a new node we introduce into the graph. This makes the number of nodes at most $m + n$.

Now, let f be a flow given to us. We will try to see if we can improve this flow. We will define the *residual capacity* $c_f : V \times V \rightarrow \mathbb{R}_0^+$ as follows.

$$c_f(u, v) = \begin{cases} c(u, v) - f(u, v) & \text{if } (u, v) \in E \\ f(v, u) & \text{if } (v, u) \in E \\ 0 & \text{otherwise} \end{cases}$$

Basically, what this does is that, if there is any flow through the edge, you remove the flow from the capacity and add an edge in the opposite direction with the value of the flow. The reason we do this is because the flow we picked thus far might not be the correct flow, and this formulation allows us to undo changes that we have done. The residual capacity $c_f(u, v)$ represents how much flow we can send from u to v in addition to the flow f .

We define G_f to be a residual network defined with respect to f , where $V(G_f) = V(G)$ and $(u, v) \in E(G_f)$ if $c_f(u, v) > 0$. Figure 2 shows G with the residual edges.

We will show that, if there is a path from s to t in G_f , then f is not a max flow. If no such path exists, that f is a max flow.

Lemma 6.1. If t is not reachable from s in G_f , then f is a maximum flow.

Proof. Let S be the set of nodes reachable from s in G_f and $T = V \setminus S$. There are no edges in G_f from S to T since the nodes in T are not reachable from s . Note that (S, T) defines an $s - t$ cut. Now consider any $v \in S, w \in T$. We have $c_f(v, w) = 0$ since (v, w) is not an edge in G_f . There are three cases:

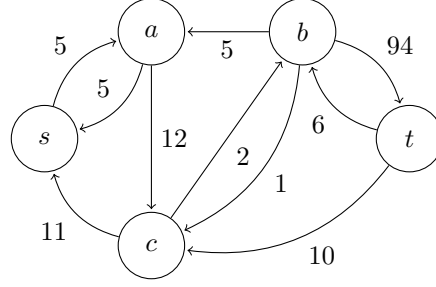


Figure 2: The residual network given the flow presented in Figure 1

1. If $(v, w) \in E$, then by definition $c_f(v, w) = c(v, w) - f(v, w) = 0 \implies c(v, w) = f(v, w)$.
2. If $(w, v) \in E$, then $c_f(v, w) = f(w, v) = 0$.
3. If $(v, w) \notin E$ and $(w, v) \notin E$, we can disregard (v, w) and (w, v) since they do not appear in any flow or cut.

Using this, and the proof in Lemma 5.1, we have

$$\begin{aligned}
 |f| &= \sum_{v \in S} \left(\sum_{x \in N_{out}(v) \cap T} f(v, x) - \sum_{y \in N_{in}(v) \cap T} f(y, v) \right) \\
 &= \sum_{v \in S} \sum_{x \in N_{out}(v) \cap T} f(v, x) \text{ [from case 2 the second term is 0]} \\
 &= \sum_{v \in S} \sum_{x \in N_{out}(v) \cap T} c(v, x) \text{ [from case 1]} \\
 &= \|S, T\|
 \end{aligned}$$

Thus, we show that the flow is equal to the cut. From Corollary 5.1 we know that f is a maximum flow, and $\|S, T\|$ is a min cut. \square

Lemma 6.2. If G_f has a path from s to t , we can modify f to f' such that $|f| < |f'|$.

Proof. Pick a path P from s to t in G_f , and consider the edge of minimum capacity on the path. Let that capacity be F . Then we can increase our flow by F . For each edge in P , if $c_f(v, w)$ is the right direction (i.e. there is an edge $(v, w) \in E(G)$), then we can increase our flow on this edge by F . If $c_f(v, w)$ is in the opposite direction (i.e. $(w, v) \in E(G)$), then we can decrease the flow on this edge by F . In effect, we are “undoing” the flow on this edge. By doing so, we have increased our flow by F .

As an example, consider Figure 2 again. The path $s \rightarrow a \rightarrow c \rightarrow b \rightarrow t$ is a path with minimum capacity 2. Therefore, we can update our flow and push additional 2 units of flow, resulting in a flow of 18.

Formally, Let $s = x_0 \rightarrow x_1 \rightarrow \dots \rightarrow x_k = t$ be a simple path P in G_f , and let $F = \min_i c_f(x_i, x_{i+1})$. Define a new flow f' where

$$f'(u, v) = \begin{cases} f(u, v) + F & \text{if } (u, v) \in P \\ f(u, v) - F & \text{if } (v, u) \in P \\ f(u, v) & \text{otherwise} \end{cases}$$

We now need to show that f' is a flow. The capacity constraints are satisfied because for every $(u, v) \in E$,

1. If $(u, v) \in P$, then $0 \leq f(u, v) + F \leq f(u, v) + c_f(u, v) = f(u, v) + c(u, v) - f(u, v) = c(u, v)$

2. If $(v, u) \in P$, then $f(u, v) - F \leq f(u, v) \leq c(u, v)$ and $f(u, v) - F \geq f(u, v) - c_f(v, u) = 0$.
3. Otherwise, $f(u, v)$ is from the original flow f .

The conservation constraints are also satisfied: Recall that P is a simple path. Thus, for every $v \in V \setminus \{s, t\}$, P uses 0 or two edges incident on v . If P uses 0 edges on v , then flow values of the edges incident on v have not changed when going from f to f' . Thus, suppose that P uses two edges (x, v) and (v, y) incident on v . Because in G_f some edges appear in the opposite direction compared to G , we need to consider a few cases.

1. (x, v) and (v, y) are both in the same direction (an edge into v and an edge out of v); the flow into v increases by F and the flow out of it also increases by F .
2. (x, v) and (v, y) are both in the opposite direction ($(v, x), (y, v) \in E$); the flow into v decreases by F and the flow out of it also decreases by F .
3. (x, v) is in the correct direction and (v, y) is in the opposite direction. Then the flow into V changes by $F - F = 0$.
4. (x, v) is in the opposite direction and (v, y) is in the correct direction. Then the flow out of V changes by $F - F = 0$.

Finally, note that we increase our flow by F . Consider the edge (s, x_1) in P . If $(s, x_1) \in E$, the flow out of s increases by F . If $(x_1, s) \in E$, the flow into s decreases by F . By our definition of G_f , it must be that $F > 0$, and we get that $|f'| > |f|$. \square

From this, we can construct an algorithm to find the maximum flow. Starting with some arbitrary flow of the graph, construct the residual network, and check if there is a path from s to t . If there is a path, update the flow, construct the new residual graph and repeat. Otherwise, we have found the max flow.

A path from s to t in the residual graph is called an *augmenting* path, and pushing flow through it to modify the current flow is referred to as *augmenting* along the path.

Algorithm 1: maxflow(G, s, t)

```

 $f \leftarrow$  all zeroes flow;
 $G_f \leftarrow G$ ;
while  $t$  is reachable from  $s$  in  $G_f$  (check using DFS) do
     $P \leftarrow$  path in  $G_f$  from  $s$  to  $t$ ;
     $F \leftarrow$  min capacity on  $P$ ;
     $f \leftarrow f'$  as defined in Lemma 6.2;
    Update  $G_f$  to correspond to new flow;
return  $f$ ;

```

The run time of this algorithm is bounded by the number of times we update our flow. If the edge capacities are all integers, we can increase the flow by at least 1 each time we update our flow. Therefore, the runtime is $O(|f|m)$ where $|f|$ is the value of the max flow. If we have rational edge capacities, then we can multiply all edge capacities by a factor to make them all integers. However, the runtime blows up by that factor as well. If we have irrational edge capacities, then the algorithm is no longer guaranteed to terminate. So we have a problem.

We will save the day in the next sections. Algorithm 1 is called the Ford-Fulkerson method. It is actually part of a family of algorithms that depend on how the path P between s and t in G_f is selected. One can obtain P via DFS, BFS, or any other method for selecting paths. It turns out that two methods work particularly well: the shortest path method and the fattest path method. The shortest path method is known as the Edmonds-Karp algorithm or Dinic's algorithm. In this class you are only required to know the above implementation and the running time of the Edmonds-Karp algorithm, but we have included the details of these two improvements for the interested student.

The fattest path method This method finds a path between s and t that maximizes $\min_{e \in P} c_f(e)$ among all $s - t$ paths P . Finding such a path can be done in $O(m + n)$ time by a clever mix of linear time median-finding and DFS.

The shortest path method (the Edmonds-Karp algorithm/Dinic's algorithm) This method picks the path between s and t using BFS, thus picking a path that minimizes the number of edges. Finding such a path also runs in $O(m)$ time: BFS takes $O(m + n)$ to explore the whole graph, but since we only care about the vertices reachable from s this is $O(m)$ time. The total run time is $O(nm^2)$.

Since both methods of selecting a path run in linear time, the main question becomes, how many iterations does Ford-Fulkerson perform? We will answer these questions below in the next section.

7 Running time of various implementations of Ford-Fulkerson

NOTE: we did not discuss the details of this section in class, but it's in the notes for the interested reader.

7.1 The fattest path version of Ford-Fulkerson

In this section we will show that the fattest path method results in a runtime of $O(m(m+n) \log |f|)$ when run on a graph with integer capacities. Thus, when rational capacities are converted to integers by multiplying by N , we get a runtime of $O(m(m+n)(\log |f| + \log N))$ for rational capacities. Thus the effect of large N is mitigated. This method does not solve the issues when the capacities can be irrational.

To show the runtime, we prove a main claim that states that after each iteration of the algorithm, the maximum flow value in G_f goes down by a factor of $(1 - 1/m)$. This max flow value starts as $|f|$ since $G_f = G$ in the beginning of the algorithm, and ends at 0 as in the end s and t are disconnected.

Claim 1 (Main). Let f' be the max flow in G_f . Then after one iteration of Ford-Fulkerson on G_f , the max flow value becomes $\leq |f'|(1 - 1/m)$.

Proof. Let P be the fattest path from s to t in G_f . Let $F = \min_{e \in P} c_f(e)$. Let S be the nodes reachable from s in G_f via paths composed of edges with residual capacities $> F$. Thus, any edge (x, y) of G_f with $x \in S$, $y \notin S$ must have $c_f(x, y) \leq F$. In particular, this means that the size of the cut between S and $V \setminus S$ is $\sum_{x \in S, y \in V \setminus S} c_f(x, y) \leq mF$. Thus, the size of the min s - t cut in G_f is at most mF .

By the max-flow-min-cut theorem from last lecture, the size of the min $s - t$ cut is at least the size of the max-flow $|f'|$ in G_f , and so $|f'| \leq mF$. Thus $F \geq |f'|/m$.

Now, when we augment (push flow) along P , the flow in G increases by F , while the flow in G_f decreases by F . Thus, the new flow in G_f after augmenting along P becomes $|f'| - F \leq |f'|(1 - 1/m)$. \square

Now that the main claim has been proven, we can conclude with a discussion of the runtime. Consider how the max flow value in G_f evolves after t iterations. It starts as $|f|$ (where f is the max flow in G) and then after t iterations is

$$\leq |f|(1 - 1/m)^t.$$

If $t = m \ln |f|$, we get that the max flow value in G_f is

$$\leq |f|((1 - 1/m)^m)^{\ln |f|} < |f|(1/e)^{\ln |f|} = 1.$$

Since all the capacities are integers, all the residual capacities are also integers, and so the max flow value in G_f is an integer. Since it is < 1 , it must be 0. Hence after $m \ln |f|$ iterations, the max flow value in G_f is zero, s and t are disconnected and the computed flow in G is maximum. The runtime is $O((m+n)m \log |f|)$.

7.2 The shortest path version of Ford-Fulkerson

Here we analyze running Ford-Fulkerson using BFS to find a path between s and t in G_f .

With each augmentation along a path P in G_f , at least one edge is removed from G_f , namely the edge with residual capacity $F = \min_{e \in P} c_f(e)$. The main claim that we need to prove the runtime is that the number of times an edge can be removed from G_f is small. Since each iteration of the algorithm causes at least one removal, the main lemma will show that the number of iterations is small and hence the runtime is small as well.

Claim 2 (Main). Fix any (u, v) that is ever an edge in G_f . Then the number of times that (u, v) can disappear from G_f is at most $n/2$.

Once this claim is proven, we would get that the total number of edge disappearances is at most $mn/2$ and hence the number of iterations of the algorithm is also $\leq mn/2$. Because of this, the algorithm runtime is $O((m+n)mn)$.

To prove the claim, we will need a useful lemma (see below) that shows that as G_f evolves through the iterations, for any v , the (unweighted) distance from s to v in G_f cannot go down. Let's begin with some notation. Let G_f^i be the residual network after the i th iteration of the algorithm; $G_f^0 = G$. For a vertex v , let $d_i(v)$ be the (unweighted) distance from s to v in G_f^i .

Lemma 7.1. For all $i \geq 1$, and all $v \in V$, $d_{i-1}(v) \leq d_i(v)$.

Proof. Fix i . We will prove the statement for i by induction on $d = d_i(v)$.

The inductive hypothesis is that for all d and all v with $d_i(v) = d$, $d_{i-1}(v) \leq d_i(v)$. The base case is $d = 0$. We note that if $d_i(v) = 0$, then $v = s$ since we view G_f^i as an unweighted graph. But then we also have $d_{i-1}(s) = 0 \leq d_i(s)$.

For the induction, let's assume that the inductive hypothesis holds for $d - 1$, i.e. that for all x with $d_i(x) = d - 1$, $d_{i-1}(x) \leq d_i(x)$. We want to show that for all v with $d_i(v) = d$, we also have $d_{i-1}(v) \leq d_i(v)$.

Consider some v with $d_i(v) = d$. Let u be the node just before v on a shortest $s - v$ path in G_f^i . Then, $d_i(u) = d_i(v) - 1 = d - 1$ and the inductive hypothesis applies to it so that $d_{i-1}(u) \leq d_i(u)$.

We consider two cases.

Case 1: $(u, v) \in G_f^{i-1}$. Then, by the triangle inequality in G_f^{i-1} , we have that $d_{i-1}(v) \leq d_{i-1}(u) + 1$. Since $d_{i-1}(u) \leq d_i(u)$, we get that

$$d_{i-1}(v) \leq d_i(u) + 1 = (d_i(v) - 1) + 1 = d_i(v).$$

Case 2: $(u, v) \notin G_f^{i-1}$. Then, since $(u, v) \in G_f^i$, we must have that (v, u) was on the $(i - 1)$ st augmenting path. Hence $d_{i-1}(u) = d_{i-1}(v) + 1$. Hence:

$$d_{i-1}(v) = d_{i-1}(u) - 1 \leq d_i(u) - 1 = d_i(v) - 2 \leq d_i(v).$$

In both cases $d_{i-1}(v) \leq d_i(v)$ and the induction is complete. \square

Now we are ready to prove the main claim.

Fix some (u, v) that is an edge in G_f at some point. Let's consider two consecutive disappearances of (u, v) . Suppose that $(u, v) \in G_i$ but $(u, v) \notin G_{i+1}$. If after this disappearance (u, v) had another one later on, then at some point (u, v) must have appeared in G_f again. Let j be the first iteration after i so that the j th augmenting path made (u, v) appear in G_f^{j+1} .

Because $(u, v) \in G_f^i$ but $(u, v) \notin G_f^{i+1}$, (u, v) must have been in the i th augmenting path P_i .

Because $(u, v) \notin G_f^j$ but $(u, v) \in G_f^{j+1}$, (v, u) must have been in the j th augmenting path P_j .

From this we obtain that $d_i(v) = d_i(u) + 1$ and $d_j(u) = d_j(v) + 1$. Using the fact that $j > i$ and the key lemma from above we obtain

$$d_j(u) = d_j(v) + 1 \geq d_i(v) + 1 = d_i(u) + 2.$$

Thus, between (u, v) 's disappearance and its next reappearance, the distance from s to u increased by $+2$. Hence between any two consecutive disappearances the distance to u increases by ≥ 2 . The distance starts as ≥ 0 and can be $\leq n - 1$ before becoming ∞ . Thus the total number of disappearances of (u, v) is $\leq n/2$. This completes the proof of the main claim and the proof of the runtime.

8 Applications

We wrap up by talking about some applications of the Ford-Fulkerson algorithm.

8.1 Bipartite perfect matching

Let $G = (V, E)$ be an undirected, unweighted *bipartite graph*: the set of vertices is partitioned into V_1 and V_2 so that there are no edges with two endpoints entirely in V_1 or entirely in V_2 . A matching in G is a collection of edges, no two of which share an end point. A perfect matching is a matching M such that every node in V has exactly one incident edge in M . In order for G to have a perfect matching, we need that $|V_1| = |V_2|$. The perfect matching problem is, given a bipartite graph G with $|V_1| = |V_2| = n$ and on m edges, determine whether G has a perfect matching.

We will solve the bipartite perfect matching problem by creating an instance of max flow and using Ford-Fulkerson's algorithm.

Given $G = (V_1 \cup V_2, E)$, direct all the edges in E from V_1 to V_2 . Add two extra nodes s and t . Add (directed) edges from s to every node in V_1 and from every node of V_2 to t . In this new graph H , let all the edge capacities be 1 and then run Ford-Fulkerson's algorithm to compute the max flow.

Suppose that G has a perfect matching M . Then, H has max flow value $n = |V_1| = |V_2|$. This is because we can set $f(e) = 1$ for every $e \in M$, all the edges out of s and all the edges out of t . All other flow values are 0. The capacity constraints are trivially satisfied. The flow conservation constraints are satisfied since for every $x \in V_1$ there is exactly one edge (s, x) into x that has flow 1, and exactly one edge $(x, y) \in M$ with flow 1; similarly for every $x \in V_2$ there is exactly one edge (x, t) out of x that has flow 1, and exactly one edge $(y, x) \in M$ with flow 1.

Suppose now that Ford-Fulkerson returns a flow f of value n . Hence $f(s, x) = f(y, t) = 1$ for all $x \in V_1, y \in V_2$. Because Ford-Fulkerson causes all flow values on the edges to be integers, the flow values on all edges are either 1 or 0. Because of this, every node $x \in V_1$ gets flow of 1 going into it and a flow of 1 needs to come out so that there is a single edge (x, y) that has flow value 1 and all other edges out of x have flow value 0. Similarly, for every $y \in V_2$ there is a unique edge into y with positive flow value 1. The edges in $V_1 \cup V_2$ with positive flow through them must hence form a perfect matching.

8.2 More applications

There are many applications of max-flow and min-cut! We may talk about a few more in class if time (check the slides), and also check out Section 7.7 of Kleinberg and Tardos.