MONASH University

**FIT2004**

# Algorithms and Data Structures

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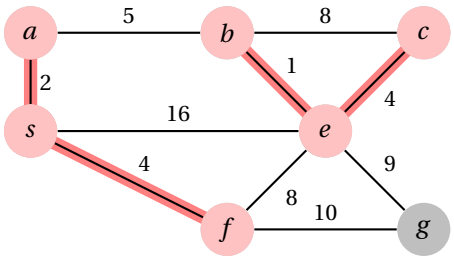


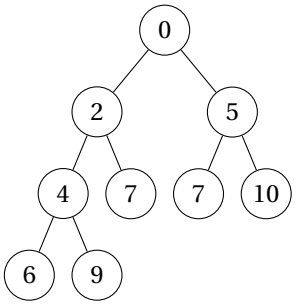


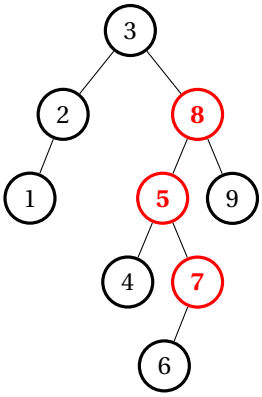


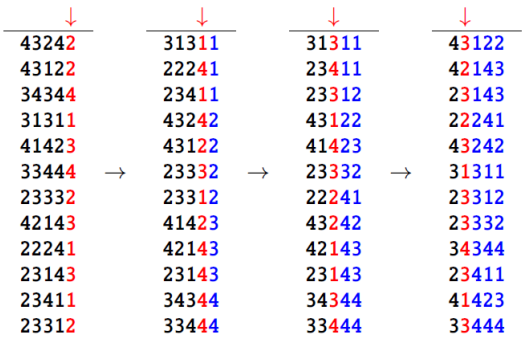


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# Chapter 1

# Analysis of Algorithms: Part I

When we write programs, we usually like to test them to give us confidence that they are correct. But testing a program can only ever demonstrate that it is wrong (if we find a case that breaks it). To prove that a program always works, we need to be more mathematical. The two major focuses of algorithm analysis are proving that an algorithm is **correct**, and determining the amount of **resources** (time and space) used by the algorithm.

**Summary: Analysis of Algorithms : Part I**

In this chapter, we cover:

- What it means to analyse an algorithm
- Correctness and termination of an algorithm
- How to prove rigorously that an algorithm is correct
- Analysing the time complexity of an algorithm
- All of the above demonstrated on binary search

**Recommended Resources: Analysis of Algorithms : Part I**

- `http://www.csse.monash.edu.au/~lloyd/tildeAlgDS/Math/`
- CLRS, Introduction to Algorithms, Pages 17 - 19, Section 2.1

## Program Verification

Program verification or correctness hinges on two main principles. We must on one hand prove that our algorithm, if it terminates always produces the correct result. On the other, we must prove that it does indeed always terminate. We will explore these issues by analysing one of the most well-known fundamental search algorithms, binary search. An implementation of binary search is shown in Algorithm 1.

Programmers, even experienced ones frequently write incorrect binary searches. Commonly they are "off-by-one" errors in which the final index reached by the search is one away from where it should have been. What if line 5 had read key > array[mid] instead? This would be a mistake, and not an easy one to find given how small of a difference it is. So how then do we

**Algorithm 1** Binary Search

```
1:  function BINARY_SEARCH(array[1..n], key)
2:      Set lo = 1 and hi = n + 1
3:      while lo < hi - 1 do
4:          Set mid = ⌊(lo + hi)/2⌋
5:          if key ≥ array[mid] then lo = mid
6:          else hi = mid
7:      end while
8:      if array[lo] = key then return lo        // key is located at array[lo]
9:      else return null        // key not found
10: end function
```

reason that this algorithm is in fact the correct one? We reason the correctness by establishing an **invariant** in the algorithm. The "key" invariant for binary search is shown below.

**Invariant: Binary Search**

If key $\in$ array, then at each iteration:

1. array[lo] $\leq$ key
2. array[hi] $>$ key. (Assume that array[n+1] $= \infty$)

Taken together, these two conditions imply that array[lo] $\leq$ key $<$ array[hi]. Combined with the sortedness of array, this implies that key (if it exists) lies within the range [lo..hi).

We can now re-interpret the binary search algorithm such that every action it takes is simply aiming to maintain these invariants. This observation can lead us to prove that the algorithm is indeed correct and that it terminates.

## Arguing correctness

When we wish to prove an algorithm's correctness via invariants, we are required to prove three things:

1. Initialisation: We must prove that the invariants hold at the beginning
2. Maintenance: We must prove that the invariants remain true throughout the algorithm
3. Termination: We must prove that the invariants at termination imply correctness of the algorithm

We will argue the proof in two parts. First we will show show binary search is correct if the key that we are searching for is in the array. Then we will prove that it is correct when the key is not in the array.

**Case 1: key $\in$ array**

We must first argue that the invariants established above are correct when the algorithm begins. Once established, we subsequently argue that the invariants are maintained throughout the algorithm. When we first begin, we initialise lo = 1, hi = $n+1$, so:

1. If key $\in$ array, since the array is sorted, lo = 1 implies that array[lo] is the minimum element, and hence array[lo] $\leq$ key.
2. If we take array[n+1] = $\infty$, then since hi = n + 1, array[hi] > key.

Therefore the invariant is true at the beginning of the binary search algorithm. As we perform iterations of the main loop of the binary search, what happens to this invariant? At each step, we compute mid = $\lfloor$(lo + hi)/2$\rfloor$ and compare array[mid] to key. The conditional statement in the loop then enforces the invariant.

1. If key $\geq$ array[mid], then after setting lo = mid, we will still have array[lo] $\leq$ key
2. If key < array[mid], then after setting hi = mid, we will still have array[hi] > key.

Hence the invariant holds throughout the iterations of the loop. Therefore, if the loop terminates, it is true that array[lo] $\leq$ key < array[hi]. Since the condition for the loop to terminate is that lo $\geq$ hi - 1, combined with the previous inequality, it must be true that lo = hi - 1. Therefore if key exists in array at all, it must exist at position lo, and hence the binary search algorithm correctly identifies whether or not key is an element of array.

**Case 2: key $\notin$ array**

Since key is not in the array, provided that the algorithm terminates, regardless of the value of lo, array[lo] $\neq$ key and hence the algorithm correctly identifies that key is not an element of array.

## Arguing termination

We have argued that binary search is correct **if it terminates**, but we still need to prove that the algorithm does not simply loop forever, otherwise it is not correct. Let us examine the loop condition closely. The loop condition for binary search reads lo < hi - 1, hence while we are still looping, this inequality holds. We now recall that

$$\text{mid} = \left\lfloor \frac{\text{lo} + \text{hi}}{2} \right\rfloor.$$

**Theorem: Finiteness of Binary Search**

If lo < hi - 1, then

$$\text{lo} < \text{mid} < \text{hi}$$

**Proof**

Since mid is the floor of (lo + hi)/2, it is true that

$$\frac{\text{lo}+\text{hi}}{2}-1<\text{mid}\leq\frac{\text{lo}+\text{hi}}{2}.$$

Multiplying by two, we find

$$\text{lo}+\text{hi}-2<2\times\text{mid}\leq\text{lo}+\text{hi}.$$

Since lo < hi-1, we have lo ≤ hi-2. We replace hi-2 with lo on the left most term in the inequality.

$$2\times\text{lo}<2\times\text{mid}\leq\text{lo}+\text{hi}.$$

Next, we add 1 to the right most term.

$$2\times\text{lo}<2\times\text{mid}<\text{lo}+\text{hi}+1.$$

Since lo < hi-1, we have lo+1 < hi. We replace lo+1 with hi on the right most term.

$$2\times\text{lo}<2\times\text{mid}<2\times\text{hi}.$$

and hence

$$\text{lo}<\text{mid}<\text{hi},$$

as desired.

Since this is true, and we always set either lo or hi to be equal to mid, it is always the case that at every iteration, the interval [lo..hi) decreases in size by at least one. The interval [lo..hi) is finite in size, therefore after some number of iterations it is true that lo ≥ hi - 1. Therefore the loop must exit in a finite number of iterations and hence the binary search algorithm terminates in finite time.

## Complexity Analysis

We have proven that the binary search algorithm terminates, and that it terminates with the correct answer. The only thing left to do is to prove that it terminates **fast**. We can express the number of operations performed by the binary search algorithm $T(n)$ as a function of the size $n$ of the input data. The number of operations taken by the binary search algorithm can be expressed as

$$T(n)=\begin{cases}T\left(\frac{n}{2}\right)+a & \text{if } n>1,\\ b & \text{if } n=1,\end{cases} \tag{1.1}$$

where $a$ is some constant number of operations that we perform each step, and $b$ is some constant number of operations required at the end of the algorithm.

**Theorem: Time Complexity of Binary Search**

The recurrence relation (1.1) has the explicit solution

$$T(n) = a\log_2(n) + b$$

**Proof**

We will prove that $T(n) = a\log_2(n) + b$ by induction on $n$.

**Base case:**

Suppose $n = 1$, then $a\log_2(n) + b = b$ which agrees with our definition of $T(n)$.

**Inductive step:**

Suppose that for some $n$, it is the case that $T\left(\frac{n}{2}\right) = a\log_2\left(\frac{n}{2}\right) + b$. It is then true that

$$\begin{aligned} T(n) &= T\left(\frac{n}{2}\right) + a \\ &= a\log_2\left(\frac{n}{2}\right) + b + a \\ &= a(\log_2(n) - \log_2(2)) + b + a \\ &= a\log_2(n) - a + b + a \\ &= a\log_2(n) + b \end{aligned}$$

as desired. Hence by induction on $n$, it is true that

$$T(n) = a\log_2(n) + b.$$

Given this, we can conclude that the time complexity of binary search is $O(\log(n))$.

## Solutions to common recurrence relations

When analysing the time and space complexity of our algorithms, we will frequently encounter some very similar recurrence relationships whose solutions we should be able to recall.

### Logarithmic Complexity

The solution to the recurrence relation

$$T(n) = \begin{cases} T\left(\frac{n}{2}\right) + a & \text{if } n > 1, \\ b & \text{if } n = 1, \end{cases}$$

is given by

$$T(n) = a\log_2(n) + b.$$

This is the complexity of binary search that we proved above.

**Linear Complexity**

The solution to the recurrence relation

$$T(n)=\begin{cases} T(n-1)+a & \text{if} n>0, \\ b & \text{if} n=0, \end{cases},$$

is given by

$$T(n)=a\,n+b,$$

**Superlinear Complexity**

The solution to the recurrence relation

$$T(n)=\begin{cases} 2\,T\left(\frac{n}{2}\right)+a\,n & \text{if } n>1, \\ b & \text{if} n=1, \end{cases}$$

is given by

$$T(n)=a\,n\log(n)+b\,n.$$

This is the complexity of many divide and conquer sorting algorithms, such as Mergesort.

**Quadratic Complexity**

The solution to the recurrence relation

$$T(n)=\begin{cases} T(n-1)+c\,n & \text{if } n>0, \\ b & \text{if} n=0, \end{cases}$$

is given by

$$T(n)=c\left(\frac{n(n+1)}{2}\right)+b.$$

This recurrence shows up for example, as the worst-case complexity of Quicksort.

**Exponential Complexity**

The solution to the recurrence relation

$$T(n)=\begin{cases} 2\times T(n-1)+a & \text{if } n>0, \\ b, & \text{if } n=0, \end{cases},$$

is given by

$$T(n)=(a+b)\times 2^n-a.$$

# Asymptotic Notation

When analysing the complexity of algorithms, we typically concern ourselves only with the order of magnitude of the running time for large values of $n$. We express time and space complexities in terms of *asymptotic notation*, with which you should be familiar. We use the following notation throughout the course.

## Big-O notation

Big-O is the notation that we will use most frequently. Informally, big-O notation denotes an **upper bound** on the size of a function. That is, $f(n) = O(g(n))$ means $f(n)$ is no bigger than than order of magnitude of $g(n)$. Formally, we say that $f(n) = O(g(n))$ as $n \to \infty$ if

$$f(n) \leq c \cdot g(n) \qquad \text{for all } n \geq n_0$$

for some constants $c$ and $n_0$. This says that for values of $n$ above some threshold, $f$ is always no bigger than some constant multiple of $g$. Note that this means the behaviour of $f$ for small values of $n$ is irrelevant. Big-O notation is used to classify the runtime of algorithms by stating that they do at most a certain amount of operations.

## Big-$\Omega$ notation

Big-$\Omega$ (Omega) notation will be used once or twice throughout the course. It is a counterpart to big-O notation that denotes a **lower bound** instead of an upper bound. That is, $f(n) = \Omega(g(n))$ means that $f(n)$ is at least as big as the order of magnitude of $g(n)$. Formally, we say that $f(n) = \Omega(g(n))$ as $n \to \infty$ if

$$f(n) \geq c \cdot g(n) \qquad \text{for all } n \geq n_0,$$

for some constants $c$ and $n_0$. Note that this is equivalent to saying that $g(n) = O(f(n))$. Big-$\Omega$ notation is used to state lower bounds on the runtime of algorithms, i.e. to say that an algorithm has to do at least a certain amount of operations.

## Big-$\Theta$ notation

We will make use of big-$\Theta$ occasionally. Big-$\Theta$ denotes the combination of big-O and big-$\Omega$, both an upper bound and a lower bound. That is, $f(n) = \Theta(g(n))$ means that $f(n)$ is the same order of magnitude as $g(n)$. Formally, we say that $f(n) = \Theta(g(n))$ as $n \to \infty$ if

$$f(n) = O(g(n)) \text{ and } f(n) = \Omega(g(n)) \text{ as } n \to \infty,$$

or equivalently if

$$f(n) = O(g(n)) \text{ and } g(n) = O(f(n)) \text{ as } n \to \infty.$$

When used to denote the running time of an algorithm, big-$\Theta$ notation implies that the amount of operations performed by the algorithm is precise, i.e. it is neither an overestimate nor an underestimate, which big-O and big-$\Omega$ notation could denote.

# Chapter 2

# Analysis of Algorithms: Part II

Invariants are a powerful tool for establishing the correctness of algorithms. Arising frequently and being of particular importance are *loop invariants*, which are invariants that are maintained by an iterative procedure (or loop) of a program. Loop invariants help us to analyse and establish the correctness of many simple sorting algorithms, which we will explore as an example.

**Summary: Analysis of Algorithms : Part II**

In this chapter, we cover:

- Using invariants to analyse algorithms
- Strong and weak loop invariants
- Analysing sorting algorithms using these invariants
- Best, average and worst-case performance of simple sorting algorithms

**Recommended Resources: Analysis of Algorithms : Part II**

- CLRS, Introduction to Algorithms, Chapter 2
- Weiss, Data Structures and Algorithm Analysis, Chapter 7
- `https://youtu.be/Kg4bqzAqRBM` - MIT 6.006 lecture on insertion & merge sort
- `https://visualgo.net/en/sorting` - Visualisation of sorting algorithms
- `http://www.csse.monash.edu.au/~lloyd/tildeAlgDS/Math/`
- `http://www.csse.monash.edu.au/~lloyd/tildeAlgDS/Sort/`

## Quadratic Sorting Algorithms

Sorting algorithms are some of the most important and fundamental routines that we will study. They are also very good case studies for the analysis of algorithms. You may be familiar with some of the quadratic ($O(n^2)$) sorting algorithms such as:

- Bubble sort
- Selection sort
- Insertion sort

You probably also know some much faster $O(n \log(n))$ sorting algorithms that we will deal with later. In this chapter, we will analyse selection sort and insertion sort, compare the two, and explore their fundamental underlying properties.

## Selection sort

The selection sort algorithm is based on the following ideas:

**Key Ideas: Selection sort**

- Consider the list to be sorted as being divided into two parts
  1. The first part consists of the part of the list that is currently sorted
  2. The remaining part consists of the elements that are yet to be sorted
- Initially, the first (sorted) part is empty, while the remaining part is the entire (to be sorted) list
- We then sort the list like so:
  1. Search the unsorted part for the smallest element
  2. Swap this smallest element with the first element of the unsorted part
  3. The sorted part is now one element longer

Expressed more concretely, an implementation of selection sort is depicted in Algorithm 2.

**Algorithm 2** Selection sort

```
1:  function SELECTION_SORT(array[1..n])
2:      for i = 1 to n do
3:          Set min = i
4:          for j = i+1 to n do
5:              if array[j] < array[min] then
6:                  min = j
7:              end if
8:          end for
9:          swap(array[i], array[min])
10:     end for
11: end function
```

Let's try to understand what is going on here more logically. At some given value of i in the main loop of the algorithm, we have the two sublists

- array[1..i-1], the sorted part
- array[i..n], the yet to be sorted part

The key strategy behind selection sort simply says to progressively make i larger while maintaining the following invariants.

**Invariant: Selection sort**

For any given value of i in the main loop of selection sort, at the beginning of the iteration, the following invariants hold:

1. array[1..i-1] is sorted
2. For any x ∈ array[1..i-1] and y ∈ array[i..n], x ≤ y

Using these invariants, arguing the correctness of selection sort is easy.

**Initial state of the invariants**

Initially, when i = 1, the sorted part of the array array[1..0] is empty, so the invariants trivially hold. Note that we will often use the notation array[1..0] (or similarly array[$n$+1..$n$]) to mean an empty array for convenience.

**Maintenance of the invariants**

At each iteration of the main loop, we seek the minimum array[j] for $i \leq j \leq n$. Since at the beginning of iteration i, it is true that array[1..i-1] ≤ array[i..$n$], the value of array[min] is no greater than any x ∈ array[1..i-1], and hence the extended sorted part array[1..i] remains sorted after swapping array[i] and array[min], so invariant 1 is maintained.

Since we are selecting array[min] as a minimum of array[i..$n$], it must be true that after swapping array[i] and array[min], that array[min] ≤ array[i+1..$n$], so invariant 2 is also maintained.

**Termination**

When the i loop terminates, the invariant must still hold, and since it was maintained in iteration i = $n$, this implies that array[1..$n$] is sorted, i.e. the entire list is sorted, and we are done.

**Time and space complexity of selection sort**

Selection sort always does a complete scan of the remainder of the array on each iteration. It is therefore not hard to see that the number of operations performed by selection sort is independent of the contents of the array. Therefore the best, average and worst-case time complexities are all exactly the same.

**Theorem: Time complexity of selection sort**

The time complexity of selection sort is $O(n^2)$.

**Proof**

The number of iterations performed is $n$ - i for each i from 1 to $n$, therefore we perform

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

total operations.

We also only require one extra variable and some loop counters, so the amount of extra space required for selection sort is constant.

| | **Best case** | **Average Case** | **Worst Case** |
|---|---|---|---|
| Time | $O(n^2)$ | $O(n^2)$ | $O(n^2)$ |
| Auxiliary Space | $O(1)$ | $O(1)$ | $O(1)$ |

## Insertion sort

Insertion sort is a very similar algorithm to selection sort, based on a similar but *weaker* invariant. The idea behind insertion sort, much like selection sort is to maintain two sublists, one that is sorted and one that is yet to be sorted. At each iteration of the algorithm, we move one new element from the yet-to-be sorted sublist into its correct position in the sorted sublist. An implementation of insertion sort might look something the code shown in Algorithm 3.

**Algorithm 3** Insertion sort

```
1:  function INSERTION_SORT(array[1..n])
2:      for i = 2 to n do
3:          Set key = array[i]
4:          Set j = i - 1
5:          while j > 0 and array[j] > key do
6:              array[j+1] = array[j]
7:              j = j - 1
8:          end while
9:          array[j+1] = key
10:     end for
11: end function
```

selection sort was based on the idea that we maintain two invariants with respect to the sorted and yet-to-be-sorted sublists. We required that the first sublist be sorted, and that the second

sublist contain elements greater or equal to those in the sorted sublist. Insertion sort maintains a weaker invariant shown below. We call the invariant weaker since it maintains a subset of the invariants that selection sort did.

**Invariant: Insertion sort**

For any given value of i in the main loop of insertion sort, at the beginning of the iteration, the following invariant holds:

1. array[1..i-1] is sorted

Let's prove that this invariant holds and is sufficient to prove that insertion sort is correct.

**Initial state of the invariant**

Again, the sorted sublist is empty at the beginning of the main loop, so the invariant holds.

**Maintenance of the invariant**

At the beginning of iteration i, the sublist array[1..i-1] is sorted. The inner while loop of insertion sort swaps the item array[j] one place to the left until array[j-1] $\leq$ array[j]. Since array[1..i-1] was originally sorted, it is therefore true that after the termination of the while loop, array[1..j] is sorted. Since the sublist array[j+1..i] was originally sorted, and for each x $\in$ array[j+1..i], we had array[j] < x, it is also true that array[j..i] is sorted. Combining these observations, we can conclude that array[1..i] is now sorted, and hence the invariant has been maintained.

**Termination**

At each iteration of the inner while loop of insertion sort, j is decremented, therefore either the loop condition j $\geq$ 2 must eventually be false, or it will be the case that array[j-1] $\leq$ array[j]. Since the loop invariant was maintained when i = $n$, it is true that array[1..$n$] is sorted, and we are done.

**Time and space complexity of insertion sort**

Unlike selection sort, insertion sort behaves differently depending on the contents of the array. Suppose we provide insertion sort with an already-sorted list. The inner loop will never iterate since it will always be true that array[j-1] $\leq$ array[j]. Therefore the only operations required by insertion sort are to perform the outer loop from from 1 to $n$, so in the best case, insertion sort only takes $O(n)$ time. In the worst case, suppose we provide an array that is sorted in reverse order. We can see that in this case, the inner while loop of insertion sort will have to loop the entire way from i to 1 since it will always be true that array[j] < array[j-1]. We observe that in this case, the amount of work done is the same as selection sort, since we perform i - 1 operations for each i from 2 to $n$. Therefore in the worst case, insertion sort takes $O(n^2)$ time.

For a random list, in the average case we will have to swap array[j] with half of the proceeding elements, meaning that we need to perform roughly half of the amount of operations as the worst case. This means that in the average case, insertion sort still takes $O(n^2)$ time. Finally, just like selection sort, the amount of extra space required is constant, since we keep only one extra variable and a loop counter.

| | **Best case** | **Average Case** | **Worst Case** |
|---|---|---|---|
| Time | $O(n)$ | $O(n^2)$ | $O(n^2)$ |
| Auxiliary Space | $O(1)$ | $O(1)$ | $O(1)$ |

# Properties of Algorithms

## Stable Sorting

A sorting algorithm is said to be *stable* if the relative ordering of elements that compare equal is maintained by the algorithm. What does this mean? Say for example that we are going to sort a list of people's names **by their length**. If multiple names have the same length, a stable sorting algorithm will guarantee that for each class of names with the same length, that their ordering is preserved. For example, if we want to sort the names `Bill`, `Bob`, `Jane`, `Peter`, `Kate` by their length, the names `Bill`, `Jane`, `Kate` all share the same length. A stable sorting algorithm will produce the following sorted list

```
Bob, Bill, Jane, Kate, Peter
```

noticing that `Bill`, `Jane`, `Kate` are relatively in the same order as the initial list. An *unstable* sorting algorithm may have shuffled the order of `Bill`, `Jane`, `Kate` while still producing a list of names that is sorted by length. Insertion sort is an example of a stable sorting algorithm. Selection sort on the other hand is not a stable sorting algorithm.

## Online Algorithms

An algorithm (sorting or otherwise) is called *online* if it can process its input sequentially without knowing it all in advance, as opposed to an *offline* algorithm which must know the entire input in advance. Insertion sort is an example of an online sorting algorithm. If you only know some of the input, you can begin to run insertion sort, and continue to read in the rest of the input while continuing to sort, and the algorithm will still work. On the other hand, selection sort is not an online algorithm, since if any new elements are added to the input, the algorithm would have to start all over.

## In-place Algorithms

There are multiple definitions of an *in-place* algorithm used by different authors. One such definition is that an algorithm is in place if it uses $O(1)$ auxiliary space. This is quite hard to satisfy, so some authors use the following definition instead. An algorithm (sorting or otherwise) is called *in place* if it does not store or copy the input into any additional data structures, but modifies the input directly to produce the output. More concretely, an algorithm is in place if it never stores more than $O(1)$ elements of the input outside of the input. Insertion sort and selection sort are both examples of in-place algorithms for both definitions.

# Chapter 3

# Fast Sorting Algorithms

Sorting is a fundamental and interesting problem in computer science. Many sorting algorithms exist, each having their own advantages and disadvantages. Sorting algorithms like selection sort and insertion sort take $O(n^2)$ time but are very easy to implement and run very fast for very small input sizes. Faster sorting algorithms exists which only take $O(n \log(n))$ time, but which may be more difficult to implement and may run slower for small lists. We will analyse some of these algorithms and also explore some interesting theoretical results regarding sorting. We will also take a look at how in many cases, integers can be sorted in just $O(n)$ time.

**Summary: Fast Sorting Algorithms**

In this chapter, we cover:

- Complexity lower bounds for sorting
- The Quicksort algorithm
- Sorting integers in linear time: Counting sort and radix sort

**Recommended Resources: Fast Sorting Algorithms**

- CLRS, Introduction to Algorithms, Chapters 6, 7, 8
- Weiss, Data Structures and Algorithm Analysis, Chapter 7
- `https://youtu.be/vK_q-C-kXhs` - MIT 18.410J lecture on Quicksort
- `https://youtu.be/Nz1KZXbghj8` - MIT 6.006 lecture on fast sorting
- `https://visualgo.net/en/sorting` - Visualisation of sorting algorithms

**Revision: Fast Sorting Algorithms**

You should be familiar from your previous studies with:

- The heapsort algorithm (revised below)
- The merge sort algorithm (revised below)

## Heapsort (Revision)

You should be familiar with the heap data structure from your previous units. If you've forgotten, here is a quick reminder:

**Definition: Binary Heap Data Structure**

The binary heap data structure can be described as follows.

- A binary heap is a complete binary tree (all levels except for the last are completely filled).
- Every element in a heap is no smaller than its children (i.e. the maximum element is at the top).

**Property: Binary Heap Data Structure**

The binary heap data structure has the following properties.

- Due to its structure, a binary heap can be represented as a flat array array[1..$n$] where the root node is array[1] and for each node array[i], its children (if they exist) are elements array[2i] and array[2i+1].
- An existing array can be converted into a heap in place in $O(n)$ time.
- A new item can be inserted into a binary heap in $O(\log(n))$ time.
- The maximum element can be removed from a binary heap in $O(\log(n))$ time.

Making use of the heap data structure, one can easily piece together the heapsort algorithm, which simply involves converting the given sequence into a max heap (*heapifiying* it) and then successively removing the maximum element and placing it at the back of the array.

**Algorithm 4** Heapsort

```
1: function HEAPSORT(array[1..n])
2:     heapify(array[1..n])
3:     for i = n to 1 do
4:         array[i] = extract_max(array[1..i])
5:     end for
6: end function
```

That's it! Of course you'll need to recall how to perform the HEAPIFY and EXTRACT_MAX operations. They are provided below for convenience.

### Time and space complexity of heapsort

Since heapsort performs one HEAPIFY which takes $O(n)$ time, and $n$ invocations of EXTRACT_MAX taking up to $O(\log(n))$ time each, the total time spent by heapsort is $O(n\log(n))$. Note that the

behaviour of heapsort is independent of the structure of the input array, so its best, average and worst-case performances are asymptotically the same. Notably however, since HEAPIFY is done in place and each element extracted is placed at the end of the array, heapsort requires only constant extra memory and hence its auxillary space complexity is $O(1)$.

There is one rare situation in which heapsort can run in just $O(n)$, when the entire input array consists of identical elements. In this case, each call to EXTRACT_MAX will take constant time since nothing has to be swapped to maintain the heap property. Heapsort is not an online algorithm since we begin by performing heapify which requires knowing the entire array. It is also not stable since the swaps made when heapifying and removing elements may move equal elements out of their relative order. It is however an in-place algorithm since heapify is in place and each call to EXTRACT_MAX places the element back into the array.

| | **Best case** | **Average Case** | **Worst Case** |
|---|---|---|---|
| Time | $O(n)$ | $O(n\log(n))$ | $O(n\log(n))$ |
| Auxiliary Space | $O(1)$ | $O(1)$ | $O(1)$ |

## Binary Heap Operations (Revision)

The standard operations on a min/max heap, implementing the priority queue abstract data type are:

1. *heapify*: Convert a given (not necessarily sorted) array into a min/max heap
2. *insert*: Insert an element into the heap
3. *remove*: Remove the min/max value from the heap

These operations are supported by two internal procedures:

1. *rise*: Move an element higher up the heap until it satisfies the heap property
2. *fall*: Move an element down the heap until it satisfies the heap property

The following pseudocode implements a max heap, i.e. a heap that pops the maximum value.

**Algorithm 5** Heapify

```
1: function HEAPIFY(array[1..n])
2:     for i = n/2 to 1 do
3:         fall(array[1..n], i)
4:     end for
5: end function
```

**Algorithm 6** Heap: Insert

```
1: function INSERT(array[1..n], x)
2:     array.append(x)
3:     n += 1
4:     rise(array[1..n], n)
5: end function
```

**Algorithm 7** Heap: Delete

```
1: function EXTRACT_MAX(array[1..n])
2:     swap(array[1], array[n])
3:     n = n - 1
4:     fall(array[1..n], 1)
5:     return array.pop_back()
6: end function
```

**Algorithm 8** Heap: Rise

```
1: function RISE(array[1..n], i)
2:     Set parent = ⌊i/2⌋
3:     while parent ≥ 1 do
4:         if array[parent] < array[i] then
5:             swap(array[parent], array[i])
6:             i = parent
7:             parent = ⌊i/2⌋
8:         else
9:             break
10:        end if
11:    end while
12: end function
```

**Algorithm 9** Heap: Fall

```
1: function FALL(array[1..n], i)
2:     Set child = 2i
3:     while child ≤ n do
4:         if child < n and array[child+1] > array[child] then
5:             child += 1
6:         end if
7:         if array[i] < array[child] then
8:             swap(array[i], array[child])
9:             i = child
10:            child = 2i
11:        else
12:            break
13:        end if
14:    end while
15: end function
```

## Merge Sort (Revision)

Merge sort is a divide-and-conquer sorting algorithm that sorts a given sequence by dividing it into two halves, sorting those halves and then merging the sorted halves back together. How does merge sort sort the two halves? Using merge sort of course! Merge sort is an example of a recursive sorting algorithm, where each half of the sequence is sorted recursively until we reach a base case (a sequence of only one element). The key part of merge sort is the merge routine, which takes two sorted sequences and intertwines them together to obtain a single sorted sequence. The merge algorithm is shown in Algorithm 10.

**Algorithm 10** Merge

```
1:  function MERGE(array1[i..end1], array2[j..end2])
2:      Set result = empty array
3:      while i ≤ end1 or j ≤ end2 do
4:          if j > end2 or i ≤ end1 and array1[i] ≤ array2[j] then
5:              result.append(array1[i])
6:              i += 1
7:          else
8:              result.append(array2[j])
9:              j += 1
10:         end if
11:     end while
12:     return result
13: end function
```

Observe that this merge routine is stable (since we write array1[i] ≤ array2[j], rather than <), and hence our merge sort implementation will also be stable. Using this merge routine, an implementation of merge sort can be expressed like this. We take two array parameters, one which is the actual array that we are sorting, and one for working space. The recursive merge sort pseudocode is shown in Algorithm 11. For convenience, we usually define an extra function that handles setting up the working array for us.

#### Time and space complexity of merge sort

Merge sort repeatedly splits the input sequence in half until it can no longer do so any more. The number of times that this can occur is $\log_2(n)$. Merging $n$ elements takes $O(n)$ time, so doing this at each level of recursion results in a total of $O(n\log(n))$ time. This is true regardless of the input, hence the best, average and worst-case performances for merge sort are equal. For space, we use an extra working array of size $n$, and an additional $O(\log(n))$ space to handle the recursion. This yields a total of $O(n)$ auxiliary space.

| | **Best case** | **Average Case** | **Worst Case** |
|---|---|---|---|
| Time | $O(n\log(n))$ | $O(n\log(n))$ | $O(n\log(n))$ |
| Auxiliary Space | $O(n)$ | $O(n)$ | $O(n)$ |

**Algorithm 11** Merge sort

```
1:  function MERGE_SORT(array[lo..hi], work[lo..hi])
2:      if hi > lo then
3:          Set mid = floor((lo + hi) / 2)
4:          MERGE_SORT(array[lo..mid], work[1..mid])
5:          MERGE_SORT(array[mid+1..hi], work[mid+1..hi])
6:          array[lo..hi] = MERGE(work[lo..mid], work[mid+1..hi])
7:      end if
8:  end function
9:
10: function MERGE_SORT(array[1..n])
11:     Set work = copy(input)
12:     MERGE_SORT(array[1..n], work[1..n])
13: end function
```

#### Enhancements of merge sort

Merge sort can also be implemented *bottom-up*, in which we eliminate the recursion all-together and simply iteratively merge together the sub-arrays of size 1, 2, 4, 8, ... $n$. This still requires $O(n)$ auxiliary working memory, but eliminates the use of the program stack (for recursion) and hence should be slightly faster. For the adventurous, there are also in-place implementations of merge sort that require only $O(1)$ space, but they are much more complicated[1].

## Complexity Lower Bounds for Sorting

Selection sort and insertion sort take $O(n^2)$ time, which is fine for very small lists, but completely impractical when $n$ grows large. Faster sorting algorithms such as merge sort, heapsort and Quicksort run in $O(n\log(n))$ time, which is asymptotically a significant improvement. A fundamentally interesting question is can we do better than this? For specially structured data with properties that we can exploit, the answer is yes. Interestingly, if we assume that the only valid operations that we can perform on an element are comparisons ($<,>,\geq,\leq,=,\neq$), we can prove that sorting can not possibly be done faster than $O(n\log(n))$.

**Theorem: Lower bound on comparison-based sorting**

Sorting in the comparison model takes $\Omega(n\log(n))$ in the worst case. In other words, any comparison-based sorting algorithm can not run faster than $O(n\log(n))$ in the worst case[a]

[a] Recall that $\Omega$ notation denotes an asymptotic lower bound, i.e. the algorithm must take **at least** this long.

To prove the lower bound, we consider a *decision tree* that models the knowledge we have about the order of a particular sequence of data after comparing individual elements. A decision tree

[1] See Nicholas Pippenger, Sorting and Selecting in Rounds, *SIAM Journal on Computing* 1987.

that represents the sorting process of a sequence of three elements in shown below. Each node corresponds to a set of potential sorted orders based on the comparisons performed so far. The leaf nodes of the tree correspond to states where we have enough information to know the fully sorted order of the sequence. An example of such a tree is shown in Figure 3.1.

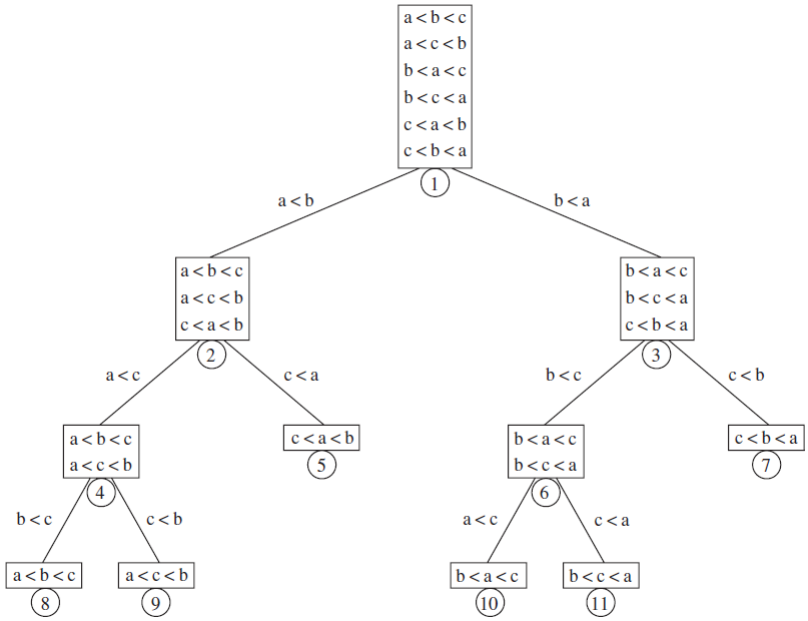



Figure 3.1: A decision tree for comparison-based sorting. Taken from Weiss, Data Structures and Algorithm Analysis in Java, 3rd ed, page 303.

**Proof:** (Not examinable in Semester Two, 2018)

We appeal to the structure of the decision tree depicted above and observe that comparing elements until we deduce the fully sorted order of a sequence is equivalent to traversing the tree until reaching a leaf node. The worst-case behaviour of any comparison based sorting algorithm therefore corresponds to the depth of the deepest leaf in the tree, i.e. the height of the tree. There are $n!$ total possible sorted orders for a sequence of $n$ elements, each of which must appear as a leaf in the tree. Let's denote the height of the tree by $h$ and observe that a binary tree of height $h$ can not have more than $2^h$ leaves. Putting this together, we have that

$$n! \leq 2^h.$$

Taking the logarithm of both sides yields

$$h \geq \log_2(n!).$$

Intuitively, one can see that $n! = O(n^n)$ and hence $\log(n!) = O(n\log(n))$. This of course only establishes an upper bound on the worst-case behaviour, not a lower bound. To

get a lower bound, let's use log laws to rewrite the quantity in question as

$$\log_2(n!) = \log_2(1 \times 2 \times 3 \times \ldots \times n) = \log_2(1) + \log_2(2) + \log_2(3) + \ldots + \log_2(n).$$

Considering just the second half of the terms, since the log function is increasing, we can write

$$\begin{aligned}
\log_2(n!) &\geq \log_2\left(\frac{n}{2}\right) + \log_2\left(\frac{n}{2}+1\right) + \ldots + \log_2(n), \\
&\geq \frac{n}{2}\log_2\left(\frac{n}{2}\right), \\
&= \frac{n}{2}(\log_2(n) - 1), \\
&= \Omega(n\log_2(n))
\end{aligned}$$

which establishes the desired lower bound. Hence the height of the tree is at least

$$h = \Omega(n\log(n)),$$

which shows that sorting in the comparison model takes $\Omega(n\log(n))$ time.

## Quicksort

Quicksort is perhaps the most well-known divide and conquer algorithms for sorting. Quicksort follows these key ideas to sort an array.

**Key Ideas: Quicksort**

- Select some element of the array, which we will call the *pivot*
- Partition the array so that all items less then the pivot are to its left, all elements equal to the pivot are in the middle, and all elements greater than the pivot are to its right
- Quicksort the left part of the array (elements less than the pivot)
- Quicksort the right part of the array (elements greater than the pivot)

The key ideas are very simple. The two major components to correctly (and efficiently) implementing Quicksort are the partitioning algorithm (how do we move elements lesser/greater than the pivot to the left/right efficiently?) and how we choose to select our pivot element.

### The partitioning problem

The partitioning problem is central to Quicksort. The choice of partitioning algorithm affects whether the algorithm is in place and whether it is stable, and can also influence the worst-case

time complexity.

### Naive partition algorithm

The naive partitioning algorithm simply partitions the array into three temporary arrays, one for elements that are less than the pivot, one for elements that are greater than the pivot, and one for elements equal to the pivot. Naive partitioning is shown as Algorithm 12

**Algorithm 12** Naive partitioning

```
1:  function PARTITION(array[lo..hi], pivot)
2:      Set left = empty array        // Store elements less than the pivot
3:      Set pivots = empty array      // Store elements equal to the pivot
4:      Set right = empty array       // Store elements greater than the pivot
5:      for i = lo to hi do
6:          if array[i] < pivot then left.append(array[i])
7:          else if array[i] = pivot then pivots.append(array[i])
8:          else right.append(array[i])
9:      end for
10:     array[lo..hi] = left + pivots + right      // Concatenate the arrays
11:     return length(left) + ⌈length(pivots)/2⌉   // Return the position of the middle pivot
12: end function
```

Naive partitioning takes $O(n)$ time and is stable, which are both nice properties. However, naive partitioning is not in place since it stores all $n$ elements in new arrays, using $O(n)$ space. Creating extra arrays means that the algorithm will be slower in practice than alternatives.

### Hoare partition algorithm

The Hoare partition algorithm is the original partitioning algorithm described by C.A.R. Hoare, the inventor of Quicksort. Hoare's partitioning scheme maintains two indices that begin at the start and end of the subarray, which move towards each other while swapping elements that are on the wrong side of the pivot. An implementation of Hoare's partitioning scheme is shown in Algorithm 13. Note that the Hoare partitioning scheme assumes that the pivot is the first element of the range, so our first step is to swap the pivot to the first location so that we can handle more general pivot selection rules later.

The Hoare partitioning scheme is in place and can be shown to be very efficient in practice. Its main disadvantage compared to the naive scheme is that it is no longer stable.

### Dutch National Flag partition algorithm (Not examinable in Semester Two, 2018)

One disadvantage of the Hoare scheme described above is that it can perform very badly when there are many elements that are equal to the pivot. All elements equal to the pivot will end up in the left side of the partition, which will be very imbalanced if many (or possible even all) elements are equal to the pivot. One way to fix this is to add a post-processing step to the partitioning algorithms that scans the partition and identifies the interval of elements equal to the

**Algorithm 13** Hoare partitioning

```
1:  function PARTITION(array[lo..hi], array[p])   // array[p] is a reference to the pivot element
2:      swap(array[lo], array[p])   // Move the pivot to the front of the array
3:      Set i = lo, j = hi
4:      while i ≤ j do
5:          while i ≤ j and array[i] ≤ p do i = i + 1
6:          while i ≤ j and array[j] > p do j = j - 1
7:          if i ≤ j then swap(array[i], array[j])   // swap elements on the wrong side
8:      end while
9:      swap(array[lo], array[j])   // swap the pivot into the correct position
10:     return j   // Return the position of the pivot
11: end function
```

pivot. These elements can then all be ignored in the subsequent recursive phases of Quicksort. An alternative partitioning scheme that accounts for this is the so called *Dutch National Flag* (DNF) scheme proposed by Edsger Dijkstra. The DNF scheme partitions the array into three sections $< p$, $= p$, and $> p$ in place. Only the $<$ and $>$ subarrays then need to be recursed on. Dijkstra described the partitioning scheme by phrasing it in terms of the following problem.

**Problem Statement**

Given an array of $n$ objects (array[1..$n$]) coloured **red**, **white** or **blue**, sort them so that all objects of the same colour are together, with the colours in the order **red**, **white** and **blue**.

The connection to the Quicksort partitioning problem should be quite clear: The **red** items correspond to elements less than the pivot, the **white** items correspond to elements equal to the pivot, and the **blue** items correspond to elements greater than the pivot. To solve the DNF problem, we maintain three pointers, lo, mid, and hi, such that the following invariant is held.

**Invariant: Dutch National Flag Partitioning Problem**

Maintain three pointers lo, mid, hi such that,

- array[1..lo-1] contains the **red** items
- array[lo..mid-1] contains the **white** items
- array[mid..hi] contains the currently unknown items
- array[hi+1..N] contains the **blue** items

Initially, we set lo = 1, mid = 1, hi = $n$. This means that initially the entire array is the unknown section. We then iteratively move items from the unknown section into their corresponding sections while updating the pointers lo, mid, hi. At each iteration, we move the item at array[mid] (i.e. the first unknown item). There are three cases to consider:

**Case 1: array[mid] is Red:**

If array[mid] is **red**, we'd like to move it into the first section. So, we will swap array[mid] with array[lo]. This means that the **red** section is extended by one element, so we increment the lo pointer. The item originally at array[lo] was either **white**, in which case it has been moved to the end of the **white** section, so we increment mid, or the **white** section was empty, meaning we simply swapped array[lo] with itself, then we increment mid. In both situations, we see that the invariant is maintained, and the unknown section has shrunk in size by one element.

**Case 2: array[mid] is White:**

If array[mid] is **white**, then it is already where we want it to be (right at the end of **white** section) so we simply have to increment the mid pointer. This also shrinks the unknown section by one element.

**Case 3: array[mid] is Blue:**

If array[mid] is **Blue**, we want to move it into the final section, so we will swap array[mid] with array[hi]. The **Blue** section is therefore extended so we decrement the pointer. We do not move the mid pointer in this case since the array[mid] now contains what was previously the final element in the unknown section.

Psuedocode implementing the DNF partitioning scheme is shown in Algorithm 14.

**Algorithm 14** Dutch national flag partitioning

```
1:  function PARTITION(array[1..n], pivot)
2:      Set lo = 1, mid = 1, hi = n
3:      while mid ≤ hi do
4:          if array[mid] < pivot then        // Red case
5:              swap(array[mid], array[lo])
6:              lo += 1, mid += 1
7:          else if array[mid] = pivot then        // White case
8:              mid += 1
9:          else        // Blue case
10:             swap(array[mid], array[hi])
11:             hi -= 1
12:         end if
13:     end while
14:     return lo, mid
15: end function
```

Note that we return the final position of the lo and mid pointers so that we can quickly identify the locations of the three sections after the partitioning. Like Hoare, also notice that this partitioning process is unfortunately not stable.

## Implementing Quicksort

We now have the tools to implement Quicksort. Assume for now that we select the first element in the range [lo..hi] to be our pivot. We will explore more complicated pivot selection rules later. Using our partitioning functions and the fact that they return the resulting location of the pivot, Quicksort can be implemented as as shown in Algorithm 15.

**Algorithm 15** Quicksort

```
1: function QUICKSORT(array[lo..hi])
2:     if hi > lo then
3:         Set pivot = array[lo]
4:         Set mid = PARTITION(array[lo..hi], pivot)
5:         QUICKSORT(array[lo..mid-1])
6:         QUICKSORT(array[mid+1..hi])
7:     end if
8: end function
```

## Time and space complexity of Quicksort

The running time of Quicksort is entirely dependent on the quality of the pivot that is selected at each stage. Ideally, the resulting partition will be balanced (contain roughly equal amounts of elements on each side) which will minimise the depth of recursion required.

### Best-case partition

In the ideal case, the pivot turns out to be the median of the array. Recall that the median is the element such that half of the array is less than it and half of the array is greater than it. This will result in us only having $\log_2(n)$ levels of recursion since the size of the array would be halved at each level. At each level, the partitioning takes $O(n)$ total time, and hence the total runtime in the best case for Quicksort is $O(n\log(n))$.

### Worst-case partition

In the worst case, the pivot element might be the smallest or largest element of the array. Suppose we select the smallest element of the array as our pivot, then the size of the subproblems solved recursively will be 0 and $n-1$. The size 0 problem requires no effort, but we will have only reduced the size of our remaining subproblem by one. We will therefore have to endure $O(n)$ levels of recursion, on each of which we will perform $O(n)$ work to do the partition. In total, this yields a worst-case run time of $O(n^2)$ for Quicksort.

### Average case partition

On average, the partitions obtained by an arbitrary pivot will be neither a perfect median nor the smallest or largest element. This means that on average, the splits should be "okay." Our intuition should tell us that in the average case, Quicksort will take an expected $O(n\log(n))$ running time, since selecting a terrible pivot at every single level of recursion is extremely unlikely.

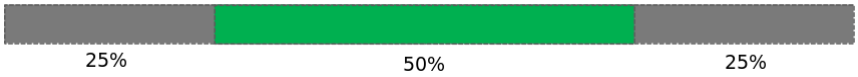
**Theorem: Average case run time for Quicksort**

The average run time for Quicksort over all possible permutations of the input array is $O(n\log(n))$.

We will present two proofs of this fact. First, an intuitive proof based on coin flips and probability, then a more rigorous proof using recurrence relations.

**Proof: Using a coin-flip argument**

Consider a random array of $n$ elements. Ideally, we would like to select a pivot that partitions the array fairly evenly. Let's define a "good pivot" to be one that lies in the middle 50% of the array, i.e. a good pivot is one such that at least 25% of the array is less than it, and 25% of the array is greater than it.




Suppose we are lucky and we select a good pivot every single time. The worst thing that can happen is that the pivot might be on the edge of the good range, i.e. we will select a pivot right on the 25$^{\text{th}}$ or 75$^{\text{th}}$ percentile. In this case, our recursive calls will have arrays of size $0.25n$ and $0.75n$ to deal with. The longest branch of the recursion tree will therefore consist of the later calls. The number of elements left after $d$ levels of recursion will be given by $0.75^d \times n = \left(\frac{3}{4}\right)^d \times n$, and hence the depth of the tree will be

$$\left(\frac{3}{4}\right)^d \times n = 1 \qquad \Longrightarrow \qquad d = \log_{\frac{4}{3}}(n)$$

Since $\log_{\frac{4}{3}}(n) = O(\log(n))$, the tree has logarithmic height. At each level of recursion we perform $O(n)$ work for the partitioning, and hence the time taken will be $O(n\log(n))$. This should not be surprising, as we already know that the best-case performance for Quicksort is $O(n\log(n))$.

We know that we can not expect to select a good pivot every time, but since the good pivots make up 50% of the array, we have a 50% probability of selecting a good pivot. Therefore we should expect that on average, every second pivot that we select will be good. In other words, we expect to need two flips of an unbiased coin before seeing heads. This means that even if every other pivot is bad and barely improves the sub-problem size, we expect that after $2 \times \log_{\frac{4}{3}}(n)$ levels of recursion to hit the base case. This means that the expected amount of work to Quicksort a random array is just twice the amount of work required in the best case, which was $O(n\log(n))$. Double $O(n\log(n))$ is still $O(n\log(n))$, hence from this we can conclude that the average case complexity of Quicksort is $O(n\log(n))$

**Proof: Using recurrence relations (Not examinable in Semester Two, 2018)**

Let us denote the time taken to Quicksort an array of size $n$ by $T(n)$. If the $k$'th smallest element is selected as the pivot, then the running time $T(n)$ will be given by

$$T(n) = n + 1 + T(k-1) + T(n-k),$$

where the terms $T(k-1)$ and $T(n-k)$ correspond to the time taken to perform the recursive calls after the pivot operation. Given this, if all partitions are equally likely to

occur, the average running time over all partitions is given by

$$T(n) = n+1+\frac{1}{n}\sum_{k=1}^{n}(T(k-1)+T(n-k)).$$

Observe that each term $T(k-1)$ appears a total of twice for each $k$ in the sum, so we have

$$T(n) = n+1+\frac{2}{n}\sum_{k=1}^{n}T(k-1).$$

Multiply this equation by $n$ to obtain

$$nT(n) = n^2+n+2\sum_{k=1}^{n}T(k-1).$$

Now substitute $n-1$ for $n$ and subtract the resulting equation from the above to find

$$nT(n)-(n-1)T(n-1) = n^2+n-(n-1)^2-(n-1)+2T(n-1).$$

Clean up with some algebra and we will get

$$nT(n) = (n+1)T(n-1)+2n.$$

Divide by $(n+1)$ and $n$ to find the recurrence

$$\frac{T(n)}{n+1} = \frac{T(n-1)}{n}+\frac{2}{n+1}.$$

Telescoping the right hand side, we obtain

$$\begin{aligned}\frac{T(n)}{n+1} &= \frac{T(n-1)}{n}+\frac{2}{n+1}.\\ &= \frac{T(n-2)}{n-1}+\frac{2}{n}+\frac{2}{n+1}\\ &= \vdots\\ &= \sum_{k=1}^{n}\frac{2}{k+1}\end{aligned}$$

where we have stopped at the base case $T(0) = 0$. Finally, using the fact that

$$\sum_{k=1}^{n}\frac{2}{k+1} = O(\log(n)),$$

(this is the asymptotic behaviour of the harmonic numbers) we obtain that

$$T(n) = (n+1)\sum_{k=1}^{n}\frac{2}{k+1} = O(n\log(n))$$

**Space complexity**

In the worst case, due to the linear number of recursive calls, we would expect that the auxiliary space required by Quicksort would be $O(n)$. This is true, but can actually be improved by making a very simple optimisation. Instead of recursively sorting the left half of the array and then the right half of the array, we can always sort the smallest half first, followed by the largest half. By sorting the smallest half first, we encounter only $O(\log(n))$ levels of recursion on the program stack, while the larger half of the partition is sorted by a tail-recursive call, which adds no overhead to the program stack. If you work in a language without tail-call optimisation, you can replace the second recursion with a loop to achieve the same effect. The complexities written below assume that such an optimisation is made.

| | **Best case** | **Average Case** | **Worst Case** |
|---|---|---|---|
| Time | $O(n\log(n))$ | $O(n\log(n))$ | $O(n^2)$ |
| Auxiliary Space | $O(\log(n))$ | $O(\log(n))$ | $O(\log(n))$ |

For the strict $O(1)$ space definition of in place, Quicksort is not in place since it requires at least $O(\log(n))$ space for recursion. Using the other definition, if we use one of the in-place partitioning schemes (Hoare or DNF) then Quicksort will also be in place, but not stable. If we use a stable partitioning scheme (such as the naive partitioning scheme), then Quicksort will be stable, but not in place.

# Sorting Integers in Linear Time

For arbitrary data, we saw before that the best possible time complexity we can achieve for comparison-based sorting is $O(n\log(n))$. However, if we make assumptions about the specific kinds of data that we are sorting, we can do better. In this section, we will focus specifically on integers, although many of these techniques can also be applied to other kinds of data, such as strings.

Suppose that we want to sort an array that consists only of 0s and 1s. This can be solved quite easily simply by counting the number of 0s and 1s in the array in linear time and then writing a new array consisting of that many 0s followed by that many 1$s$. This whole process takes linear time. This idea can be generalised to arrays of more than just 0s and 1s.

## Counting sort

Suppose we wish to sort an array that contains only integers in some fixed universe $U$. Specially, let's assume that all of the integers are in the range 0 to $u-1$. One way to achieve this is to simply do a pass over the input and count the number of occurrences of each integer. If we know that there are for example, one 0, two 1's, one 2 and three 3's, then we can immediately deduce that the sorted array is $0,1,1,2,3,3,3$ in linear time. Of course, simple naively writing out the output would not be a stable sort (indeed, any satellite data attached to the input is lost entirely), so we should instead do a second pass over the input and place each element into its

correct position. Computing the position of each element is simple. Let count[$x$] denote the number of occurrences of $x$, then the start position of the element $y$ is simply

$$\text{position}[y] = 1 + \sum_{x=0}^{y-1} \text{count}[x],$$

which can be computed in linear time in the size of the universe. Each time we place an element $y$ into its correct position, we increment position[$y$] to prepare for the next occurrence. This algorithm is called counting sort, and is shown below in Algorithm 16.

**Algorithm 16** Counting sort

```
1:  function COUNTING_SORT(array[1..n], u)
2:      Set counter[0..u-1] = [0,0,...],
3:      for i = 1 to N do
4:          counter[array[i]] += 1
5:      end for
6:      Set position[0..u-1] = [1,0,...]
7:      for value = 1 to u - 1 do
8:          position[value] = position[value-1] + counter[value-1]
9:      end for
10:     Set temp[1..n] = [0,0,...]
11:     for i = 1 to n do
12:         temp[position[array[i]] = array[i]
13:         position[array[i]] += 1
14:     end for
15:     swap(array, temp)        // Place the result into the input array
16: end function
```

This sort is stable but is not in place since we construct the answer in a separate temp array.

#### Complexity of counting sort

What is the complexity of counting sort? We are required to create and maintain the counter array of size $u$, and we do two passes over the input. This yields a time and space complexity of $O(n+u)$ in all cases.

| | **Best case** | **Average Case** | **Worst Case** |
|---|---|---|---|
| Time | $O(n+u)$ | $O(n+u)$ | $O(n+u)$ |
| Auxiliary Space | $O(n+u)$ | $O(n+u)$ | $O(n+u)$ |

This tells us that counting sort takes linear time in $n$ if and only if $u = O(n)$. It is often more informative to analyse the complexity of algorithms on integers by considering the *width* of the integers, rather than the maximum value $u$. The width of an integer is the number of bits required to represent it in binary. If we are sorting $w$-bit integers, then our universe size is

$u = 2^w - 1$. The time complexity of counting sort on $w$-bit integers is therefore $O(n + 2^w)$, which is linear in $n$ if and only if

$$w = \log(n) + O(1).$$

We will improve on this in the next section with an algorithm that can sort integers with a greater number of bits.

## Radix sort

Radix sort is a more general, non-comparison-based sort that achieves linear time for a wider class of inputs than counting sort. There are many variants of radix sort, but we will look at arguably the simplest one, least significant digit (LSD) radix sort. In essence, LSD radix sort works by sorting an array of elements one digit at a time, from the least significant to the most significant. Each digit must be sorted in a stable manner in order to maintain the relative ordering of the previously sorted digits.

**Key Ideas: Least significant digit radix sort**

- Sort the array one digit at a time, from least significant (rightmost) to most significant (leftmost)
- For each digit: Sort using a stable sorting algorithm

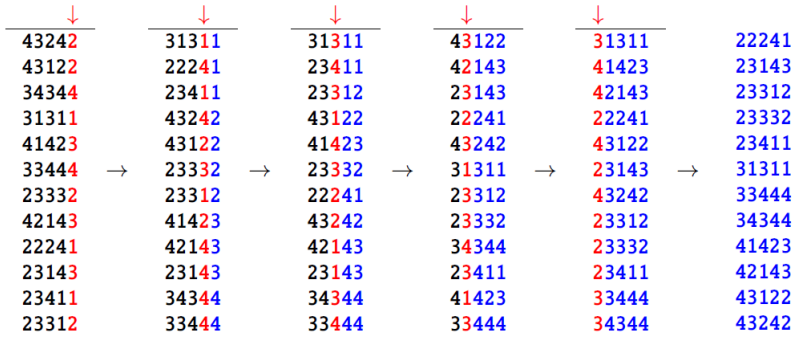



Figure 3.2: An illustration of LSD radix sort. First the numbers are sorted by their least significant digit, then their second, etc. until the most significant digit is sorted and we are finished.

Since individual digits have a very small number of possible values, we will sort the individual digits using counting sort. A visualisation of an LSD radix sort in base-10 is shown below in Figure 3.2. It is important to realise that we do not necessarily have to use their *decimal* digits to sort the elements of the array. We could have instead done radix sort with a radix (base) of 100, which would mean sorting consecutive groups of two decimal digits at a time. Using a larger radix size means less passes over the array must be made, but that more work must be done on each pass. An implementation of LSD radix sort is shown in Algorithm 17. Note that the RADIX_PASS function is simply performing counting sort on a particular digit of the input. The function GET_DIGIT($x$, $b$, $d$) computes the value of the $d^{\text{th}}$ digit in base $b$ of the integer $x$.

**Algorithm 17** Radix sort

```
1:  function RADIX_PASS(array[1..n], base, digit)
2:      Set counter[0..base-1] = [0,0,...],
3:      for i = 1 to n do
4:          counter[GET_DIGIT(array[i], base, digit)] += 1
5:      end for
6:      Set position[0..base-1] = [1,0,...]
7:      for value = 1 to base - 1 do
8:          position[value] = position[value-1] + counter[value-1]
9:      end for
10:     Set temp[1..n] = [0,0,...]
11:     for i = 1 to n do
12:         temp[position[GET_DIGIT(array[i],base,digit)]] = array[i]
13:         position[get_digit(array[i],base,digit)] += 1
14:     end for
15:     swap(array, temp)
16: end function
17:
18: function RADIX_SORT(array[1..n], base)
19:     for digit = 1 to NumDigits do
20:         RADIX_PASS(array[1..n], base, digit)
21:     end for
22: end function
```

#### Complexity of radix sort

Let's suppose that we are sorting $n$ integers that have $k$ digits in base-$b$. Radix sort will perform $k$ passes over the array, one for each digit, and perform a counting sort each time. Since we are interpreting the integers in base-$b$, the counting Sort will sort over a universe of size $b$, and hence have complexity $O(n+b)$. The total time complexity of radix sort is therefore $O(k(n+b))$, and the space complexity is just that required of counting sort, so $O(n+b)$.

So, when is radix sort linear time and how does it compare to counting sort? Suppose that we choose a constant base $b$, then the complexity of radix sort is $O(kn)$. But if our input array contains $n$ distinct integers, then the integers must have at least $k = \Omega(\log(n))$ digits. In this situation, the complexity of radix sort is at least $\Omega(n\log(n))$, so we haven't actually done any better than a comparison-based sort. We know that we can sort $\log(n)$-digit integers using counting sort in linear time, so there must be a way to make radix sort better.

Suppose again that we are sorting $w$-bit integers. Then $k$ is related to $b$ by

$$k = \frac{w}{\log(b)}.$$

For any constant $b$, we have $k = \Omega(\log(n))$, so to improve things, we have to chose the base $b$ more carefully. In terms of $w$, the time complexity of radix sort is

$$O\left(\frac{w}{\log(b)}(n+b)\right).$$

In order to make radix sort as fast as possible, we'd like the number of digits $k$ to be as small as possible, which entails using as big of a base $b$ as possible, while keeping the complexity of each counting sort at most linear. We know that counting sort will be linear provided that $b = O(n)$, so let's pick base-$n$. In this case, the complexity of radix sort becomes

$$O\left(\frac{w}{\log(n)}(n+n)\right) = O\left(\frac{w}{\log(n)}n\right).$$

From the above, we can deduce that radix sort will run in linear time in $n$ whenever $w = O(\log(n))$, which improves on counting sort by a multiplicative factor since it is only linear for $w = \log(n) + O(1)$. This implies that radix sort can sort integers in linear time provided that those integers are polynomial sized in $n$, i.e. provided that for all $x \in$ array, we have $x = O(2^{c\log(n)}) = O(n^c)$ for some constant $c$. The space complexity will be the space complexity of counting sort, which is $O(n+u)$, where $u = n$, hence it will be $O(n)$.

| | **Best case** | **Average Case** | **Worst Case** |
|---|---|---|---|
| Time | $O\left(\frac{w}{\log(n)}n\right)$ | $O\left(\frac{w}{\log(n)}n\right)$ | $O\left(\frac{w}{\log(n)}n\right)$ |
| Auxiliary Space | $O(n)$ | $O(n)$ | $O(n)$ |

The implementation of radix sort described above is stable but not in place since we use a temporary array for counting sort. Alternate implementations of radix sort can be written that are in place but not stable. In fact, it is even possible to write a stable, in-place radix sort, but it is extremely complicated and well beyond the scope of this course[2].

**Fun (Non-examinable) Fact:** We showed here two algorithms that sort integers in linear time provided that they have a bounded number of bits. Surprisingly, linear time sorting is not only possible for integers with a bounded width $w$. For integers with very large width, specifically those that have at least $w = \Omega(\log^{2+\varepsilon}(n))$ bits for some $\varepsilon > 0$, an algorithm called signature sort can sort them in linear time. It is an open research problem whether integers of any width $w$ can be sorted in linear time. The best known algorithms can sort $n$ integers of any width $w$ in $O(n\sqrt{\log(\log(n))})$ randomised, or $O(n\log(\log(n)))$ deterministic in the worst case[3].

[2] See G Franceschini, S Muthukrishnan, M Pătraşcu, Radix Sorting with No Extra Space, *ESA 2007*

[3] If interested, you should watch this lecture from MIT OpenCourseware, `https://youtu.be/pOKy3RZbSws`

# Chapter 4

# Order Statistics and Selection

Arising in many applications is the need to find the minimum, maximum or median element of a sequence. These are all special cases of a general problem called order statistics. We will consider several different cases of this problem and explore some algorithms for solving them.

**Summary: Order Statistics and Selection Algorithms**

In this chapter, we cover:

- What order statistics are
- Finding minimum and maximums
- The Quickselect algorithm
- The median of medians technique (**Not examinable in Semester Two, 2018**)

**Recommended Resources: Order Statistics and Selection Algorithms**

- CLRS, Introduction to Algorithms, Chapter 9
- Weiss, Data Structures and Algorithm Analysis, Section 10.2.3

## Order Statistics and the Selection Problem

The $k$'th order statistic of a sequence of $n$ elements is defined to be the $k$'th smallest element. For example, the first order statistic is the simply the smallest element of the sequence and the $n$'th order statistic is simply the maximum. The median element of a sequence is an element that is smaller than and larger than one half of the other elements of the sequence. In terms of order statistics, the median is the $k = (n+1)/2$ order statistic, rounding either up or down if $n$ is even. The selection problem is the problem of finding for a given sequence and a given value of $k$, the $k$'th order statistic, i.e. the $k$'th smallest element of the sequence. The easy way to solve the selection problem is of course to simply sort the sequence and then select the $k$'th element that results. Using a fast ($O(n\log(n))$) sorting algorithm would yield an $O(n\log(n))$ solution to the selection problem. In this section, we aim to explore faster algorithms for solving the selection problem.

### The easy case: finding minimums and maximums

Minimums and maximums are the simplest order statistics to find. Rather than sorting the entire sequence in $O(n\log(n))$, an obvious linear time algorithm to find the minimum and/or maximum is to simply iterate over the sequence and track the best found minimum and/or maximum so far. A possible implementation is shown in Algorithm 18.

**Algorithm 18** Select minimum

```
1: function SELECT_MIN(array[1..n])
2:     Set min = array[1]
3:     for i = 2 to n do
4:         if array[i] < min then
5:             min = array[i]
6:         end if
7:     end for
8:     return min
9: end function
```

That was rather easy, but it raises an interesting question: can we solve this problem any faster or with fewer comparisons in the general case (assuming random input?) It should not be hard to convince yourself that we can not determine the minimum with any fewer than $n-1$ comparisons, since performing less than $n-1$ comparisons leaves at least one element of the array that has never been compared to any other, which could potentially be the minimum. A more interesting problem arises if we consider the case of finding both the minimum and maximum element at the same time. Clearly, our first algorithm for finding the minimum in $n-1$ comparisons could easily be adapted to find both the minimum and maximum in $2n-2$ comparisons, but can we do better? The answer is no longer obvious since we are doing more comparisons than necessary to find either one of the minimum or maximum on its own. It turns out that we can in fact select both the minimum and maximum element of a sequence in fewer, just $\sim 1.5n$ comparisons. The trick is to just consider each pair of numbers in the input, and for each pair, to only compare the higher of the two with the current maximum, and the lower of the two with the current minimum. This results in cutting out $\frac{1}{4}$ of the comparisons which were unnecessary. The implementation shown in Algorithm 19 demonstrates this trick.

Interestingly, it is possible to prove that $1.5n$ is the smallest possible number of comparisons that are required in the worst case to select the minimum and maximum element of a sequence, so this algorithm is in fact performing the optimal number of comparisons.

## The Quickselect Algorithm

Minimums and maximums are easy to find. Of much more theoretical interest is the problem of finding the median, or indeed the general $k$'th order statistic. Remarkably, although minimums and maximums are "easy" problems that require linear time to solve, the general $k$'th order statistic problem can also be solved in $O(n)$ in the worst case, so the "hard case" and "easy case" are actually asymptotically the same difficulty!

**Algorithm 19** Select minimum and maximum

```
1:  function SELECT_MINMAX(array[1..n])
2:      Set min = array[1], max = array[1]
3:      for i = 1 + n%2 to n, step 2 do        // start at 1 if n is even, 2 if n is odd
4:          if array[i] < array[i+1] then
5:              if array[i] < min then min = array[i]
6:              if array[i+1] > max then max = array[i+1]
7:          else
8:              if array[i] > max then max = array[i]
9:              if array[i+1] < min then min = array[i+1]
10:         end if
11:     end for
12:     return min, max
13: end function
```

The Quickselect algorithm, if the name was not a massive hint already, is based on the Quicksort algorithm. Just like Quicksort, we select a pivot element, partition the array about the pivot and then repeat recursively. The major difference between Quicksort and Quickselect is that while Quicksort recursively sorts both halves of the partition, Quickselect only needs to sort the half of the partition that contains the $k$'th element, since contents of the other half does not matter. As was the case for Quicksort, pivot selection is the crucial step of the algorithm that determines whether or not the run time will be fast or slow. Using the same partition function from Quicksort, a simple realisation of Quickselect can be implemented like so.

**Algorithm 20** Quickselect

```
1:  function QUICKSELECT(array[lo..hi], k)
2:      if hi > lo then
3:          Set pivot = array[lo]
4:          Set mid = PARTITION(array[lo..hi], pivot)
5:          if k < mid then
6:              return QUICKSELECT(array[lo..mid-1], k)
7:          else if k > mid then
8:              return QUICKSELECT(array[mid+1..hi], k)
9:          else
10:             return array[k]
11:         end if
12:     else
13:         return array[k]
14:     end if
15: end function
```

Just like Quicksort though, this function has a worst-case run time of $O(n^2)$ since we might select the minimum or maximum element as the pivot and hence perform $O(n)$ levels of recursion. Luckily for us, there are strategies to avoid this sort of pathological behaviour. We will explore two such strategies: random pivot selection which results in an expected $O(n)$ run time and is

empirically the fastest strategy, and the median of medians of fives technique, which yields a guaranteed worst-case linear performance, although is not as efficient in practice.

## Randomised Pivot Selection

One of the simplest and empirically the fastest solution to avoid pathological pivot choices is to simply select the pivot randomly.

**Theorem: Randomised pivot selection**

Using randomised pivot selection, the Quickselect algorithm has expected run time $O(n)$.

**Proof:** (Not examinable in Semester Two, 2018)

Assume without loss of generality that the array contains no duplicate elements and denote by $T(n)$ the time taken by Quickselect to select the $k$'th order statistic of an array of size $n$. If the pivot selected is the $i$'th order statistic of the array, then the time taken by Quickselect will be

$$T(n,i) = n+1+\begin{cases} T(n-i) & \text{if } i<k, \\ 0 & \text{if } i=k, . \\ T(i-1) & \text{if } i>k \end{cases}$$

Averaging out over all possible pivot selections, we obtain an expected run time of

$$T(n) = n+1+\frac{1}{n}\left(\sum_{i=1}^{k-1} T(n-i)+\sum_{i=k+1}^{n} T(i-1)\times 1\right).$$

Rearranging the indices of the sums, we find that this is the same as

$$T(n) = n+1+\frac{1}{n}\left(\sum_{i=n-k+1}^{n-1} T(i)+\sum_{i=k}^{n-1} T(i)\right).$$

Since both of the sums appearing above in the bracketed expression contain a consecutive sequence of terms ending at $T(n-1)$ and there are a total of $n$ terms, they must be bounded above by the largest possible terms, so we have the inequality

$$T(n) \le n+1+\frac{2}{n}\sum_{i=n/2}^{n-1} T(i).$$

We can now prove by induction that $T(n) \le Cn = O(n)$ for some constant $C$. First, we have that $T(0) = T(0) = 1 \le Cn$ for any choice of $C \ge 1$. Now suppose that $T(i) \le Ci$ for some constant $C$ for all $i < n$ for some value of $n$. We have that

$$T(n) \le n+1+\frac{2}{n}\sum_{i=n/2}^{n-1} T(i),$$

which by our inductive hypothesis satisfies

$$T(n) \leq n+1+\frac{2}{n}\sum_{i=n/2}^{n-1} Ci.$$

Evaluating the sum using the fact that $\sum_{i=0}^{n} i = \frac{n(n+1)}{2}$, we find

$$\begin{aligned} T(n) &\leq n+1+\frac{2C}{n}\left(\frac{n(n-1)}{2}-\frac{\frac{n}{2}(\frac{n}{2}-1)}{2}\right) \\ &\leq n+1+C(n-1)-\frac{C}{2}(\frac{n}{2}-1) \\ &\leq \left(\frac{3}{4}C+1\right)n+1-\frac{C}{2} \end{aligned}$$

If we choose $C=4$ then we will have

$$T(n) \leq 4n-1 \leq 4n = Cn$$

as desired. Hence by induction on $n$, we have that $T(n)=O(n)$, completing the proof.

## Median of Medians (Not examinable in Semester Two, 2018)

The randomised pivot selection technique yields expected linear time complexity and has excellent empirical performance. From a theoretical standpoint however, it is not worst-case linear as the run time is still $O(n^2)$ if pathological pivots are selected at every single step. Despite the absolute unlikelihood of this happening, it is theoretically satisfying to come up with an algorithm that is linear in the worst case. One such linear time selection algorithm is the median of medians algorithm, which is simply a special pivot selection strategy for Quickselect. We know that if Quickselect could select the median as the pivot, then it would yield guaranteed linear run time, but of course, finding the median is precisely the problem (or one specific case of the problem) that we are trying to solve. Instead, the median of medians technique involves finding an approximate median that is good enough to guarantee linear time performance.

**Key Ideas: Median of medians**

The median of medians algorithm selects an approximate median by:

- Dividing the original list of $n$ elements into $\lceil \frac{n}{5} \rceil$ groups of size at most 5.
- Finding the median of each of these groups (just sort them since they are small)
- Finding the true median of the $\lceil \frac{n}{5} \rceil$ medians recursively using Quickselect

Using these ideas, an implementation of the median of medians technique is shown in Algo-

rithm 21. The function MEDIAN_OF_FIVE selects the true median of a small list using insertion sort.

**Algorithm 21** Median of medians

```
1:  function MEDIAN_OF_MEDIANS(array[lo..hi])
2:      if hi - lo < 5 then
3:          return MEDIAN_OF_FIVE(array[lo..hi])
4:      else
5:          Set medians = empty array
6:          for i = lo to hi, step 5 do
7:              Set j = min(i + 4, hi)
8:              Set median = MEDIAN_OF_FIVE(array[i..j])
9:              medians.append(median)
10:         end for
11:         Set n = length(medians)
12:         return QUICKSELECT(medians[1..n], ⌊(n+1)/2⌋)
13:     end if
14: end function
15:
16: function MEDIAN_OF_FIVE(array[lo..hi])
17:     INSERTION_SORT(array[lo..hi])
18:     return array[(lo+hi)/2]
19: end function
```

The recursive call made to QUICKSELECT in the median of medians algorithm must then also use MEDIAN_OF_MEDIANS to select its pivot. We call these two functions *mutually recursive* since they do not recurse directly on themselves but rather back and forth on each other.

It remains for us to prove that this technique does indeed result in guaranteed linear time performance. On the one hand, we must ensure that the pivot selected is good enough to yield low recursion depth, and on the other, we need to be convinced that finding the approximate median does not take too long and kill the performance of the algorithm.

**Theorem: Worst-case performance of the median of medians algorithm**

Quickselect using the median of medians strategy has worst case $O(n)$ performance.

**Proof**

First, we note that out of the $\frac{n}{5}$ groups, half of them must have their median less than the pivot (by definition of the median). Similarly, half of the $\frac{n}{5}$ groups must have their medians greater than the pivot. Together, we have $\frac{n}{10}$ groups whose median is less than the pivot, and $\frac{n}{10}$ groups whose median is greater than the pivot.

Since within each group of five, two elements are greater than its median and two elements are less than its median, we have transitively that in each of the $\frac{n}{10}$ groups whose median is less than the pivot, three elements that are less than the pivot, and similarly

in each of the $\frac{n}{10}$ groups whose median is greater than the pivot, three elements that are greater than the pivot. This yields a grand total of $\frac{3n}{10}$ elements that are below and above the pivot respectively.

Consequently, the median of medians lies in the 30th to 70th percentile of the data. From this, we know that the worst case of the recursive call made by Quickselect will be on a sequence of size $0.7n$. In addition to the recursive call, we also make an additional recursive call of size $0.2n$ to compute the exact median of the original $\frac{n}{5}$ medians. Adding in the linear number operations required to perform the partitioning step and to find the median of each group of 5, a recurrence relation for the amount of work done by Quickselect using the median of medians strategy is

$$T(n) = an + T(0.2n) + T(0.7n), \qquad T(0) = 0,$$

for some constant $a$. We can show that this recurrence relation has solution $T(n) \leq Cn$ for some constant $C$ by induction. First let $C$ be a constant such that $C \geq 10a$. Consider the base case

$$T(0) = 0 <= C \times 0 = 0,$$

which trivially holds. Now suppose that $T(n) \leq Cn$ for $n < N$, then we have, by substituting this inductive hypothesis

$$\begin{aligned} T(n) &= an + T(0.2n) + T(0.7n) \\ &\leq an + 0.2Cn + 0.7Cn \quad . \\ &= an + 0.9Cn \end{aligned}$$

Since we chose the constant $C \geq 10a$, we have that

$$T(n) \leq an + 0.9Cn \leq 0.1Cn + 0.9Cn = Cn,$$

and hence by induction, for all $n > 0$,

$$T(n) \leq Cn = O(n).$$

## Improving Quicksort

Finally, we note that we can use the Quickselect algorithm to improve Quicksort. If we use Quickselect to pick the median as Quicksort's pivot, which is sometimes referred to as Balanced Quicksort, we will get the minimum possible recursion depth, resulting in a guaranteed worst-case $O(n \log(n))$ performance! In practice, this strategy is outperformed by random pivot selection, but it is satisfying to see Quicksort achieve the same worst-case behaviour as heapsort and merge sort.

# Chapter 5

# Dynamic Programming: Part I

A powerful technique that we have already encountered for solving problems is to reduce a problem into smaller problems, and to then combine the solutions to those smaller problems into a solution to the larger problem. We have seen this for example in the recursive computation of Fibonacci numbers, and in the divide-and-conquer algorithms for sorting (Merge Sort and Quicksort). In some situations, the smaller problems that we have to solve might have to be solved multiple times, perhaps even exponentially many times (for example, recursive computation of the Fibonacci numbers). Dynamic programming involves employing a technique called *memoisation*, where we store the solutions to previously computed subproblems in order to ensure that repeated problems are solved only once. Dynamic programming very frequently arises in optimisation problems (minimise or maximise some quantity) and counting problems (count how many ways we can do a particular thing).

**Summary: Dynamic Programming: Part I**

In this chapter, we cover:

- The key ideas behind dynamic programming
- Memoisation applied to computing Fibonacci numbers
- The coin change problem
- The top-down approach vs. the bottom-up approach
- Reconstructing solutions to optimisation problems

**Recommended Resources: Dynamic Programming**

- CLRS, Introduction to Algorithms, Chapter 15
- Weiss, Data Structures and Algorithm Analysis, Section 10.3
- Halim, Competitive Programming 3, Section 3.5
- `https://visualgo.net/en/recursion` - Visualisation of recursion tree
- `https://youtu.be/OQ5jsbhAv_M` - MIT 6.006 lecture on DP: Part I
- `http://users.monash.edu/~lloyd/tildeAlgDS/Dynamic/`

# The Key Elements of Dynamic Programming

## Memoisation - Computing Fibonacci numbers

The essence of dynamic programming is to solve a problem by breaking it into smaller subproblems and combining the solutions of those subproblems into a solution to the greater problem. In contrast with the divide-and-conquer method which also employs the same idea, dynamic programming applies when the subproblems **overlap** and are repeated multiple times. Recall the example of computing Fibonacci numbers recursively. Fibonacci numbers are defined by recurrence relation

$$F(n) = F(n-1) + F(n-2), \qquad F(0) = 0, \quad F(1) = 1,$$

and can be computed recursively with a very simple algorithm shown in Algorithm 22.

**Algorithm 22** Recursive Fibonacci numbers

```
1: function FIBONACCI(n)
2:     if n ≤ 1 then
3:         return n
4:     else
5:         return FIBONACCI(n-1) + FIBONACCI(n-2)
6:     end if
7: end function
```

Although simple, this algorithm is extremely inefficient. What is its time complexity? Well, the amount of work taken $T(n)$ to compute the value of $F(n)$ is the sum of the times taken to compute the values of $T(n-1)$ and $T(n-2)$, so the time complexity is given by the solution to the recurrence

$$T(n) = T(n-1) + T(n-2) + c.$$

Hopefully we recognise the main piece of this recurrence, its just the Fibonacci recurrence with an added constant! The time complexity to compute $F(n)$ can therefore be shown to be $O(F(n))$. As cool as this fact is, hopefully you remember from your mathematics study, that the Fibonacci numbers grow exponentially, so this is an extremely slow algorithm. Specifically they grow asymptotically like $\varphi^n$ where $\varphi$ is the golden ratio. How does it get so bad? What exactly are we doing so wrong?

Figure 5.1 depicts what happens when we try to compute $F(n)$. $F(n)$ and $F(n-1)$ are computed once, $F(n-2)$ is computed twice, $F(n-3)$ is computed three times, $F(n-4)$ is computed five times... In general, $F(n-k)$ is computed $F(k+1)$ times, so the leaves of the call tree are computed exponentially many times, which explains why the algorithm is so slow. The solution to this problem is simple but demonstrates the most powerful, core idea of dynamic programming. Instead of allowing ourselves to compute the same thing over and over again, we will simply store the result of each computation in a table, and if we are required to compute it again, we can look it up and return it straight from the table without any recomputation. This technique is called **memoisation** (no, that is not a typo, it is actually spelled and pronounced *memo-isation*). A memoised implementation of the recursive Fibonacci number calculation is shown in Algorithm 23.

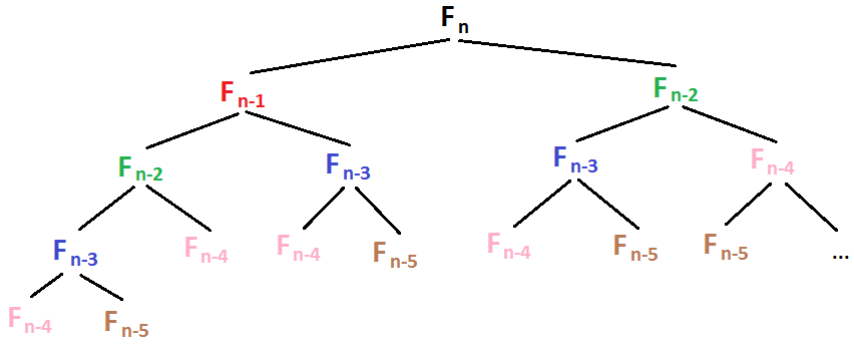



Figure 5.1: The call tree resulting from the recursive Fibonacci function for computing $F_n$.

**Key Ideas: Memoisation**

Memoisation is the process of remembering the solutions to previously computed subproblems and storing them in a table for later lookup. If the same subproblem needs to be computed multiple times, it need only be computed once, and then can be subsequently looked up from the memo table at no additional cost.

Dynamic programming solves problems that exhibit overlapping or repeated subproblems by using memoisation to avoid doing redundant work.

**Algorithm 23** Memoised Fibonacci numbers

```
1:  function FIBONACCI_MEMO(n)
2:      if n ≤ 1 then return n        // The base case
3:      if memo[n] = null then        // Compute it for the first time
4:          memo[n] = FIBONACCI_MEMO(n-1) + FIBONACCI_MEMO(n-2)
5:      end if
6:      return memo[n]
7:  end function
8:
9:  function FIBONACCI(n)
10:     Set memo[0..n] = null
11:     return FIBONACCI_MEMO(n)
12: end function
```

We store the Fibonacci numbers that have been computed in the memoisation table memo, and return straight from the table whenever we encounter a problem that we already have the solution to. The initial value of **null** in the table is used to indicate that we have not computed that number yet. If we were planning on computing lots of Fibonacci numbers, we could even keep the memo table between calls. Since each call to FIBONACCI_MEMO takes constant time, each problem is never computed more than once, and there are $n$ subproblems, the total time complexity of this implementation is $O(n)$.

The approach that we have implemented above is an example of "top-down" dynamic programming since we first ask for the solution to the largest problem and recursively ask for the solutions to smaller problems while filling in the memoisation table. An alternative implementation would be to start from the smaller problems and work our way up to the big problems. This would be the "bottom-up" approach. A bottom-up version of computing Fibonacci numbers is shown in Algorithm 24.

**Algorithm 24** Bottom-up Fibonacci numbers

```
1: function FIBONACCI(n)
2:     Set fib[0..n] = 0
3:     fib[1] = 1
4:     for i = 2 to n do
5:         fib[i] = fib[i-1] + fib[i-2]
6:     end for
7:     return fib[n]
8: end function
```

We will explore the differences between the top-down and bottom-up approaches soon.

## Optimal substructure - The coin change problem

A classic and very illustrative example of dynamic programming is the coin change problem. Suppose we have currency with denominations $c_1, c_2, ...c_n$ and we wish to make exactly $\$V$. There might be many ways to make this dollar amount. The coin change problem is to find the one that uses the fewest coins possible. For example, if the denominations are $\$1, \$5, \$6, \$9$ then the minimum amount of coins required to make \$13 is three, using two \$6 coins and one \$1 coin.

### Identifying the subproblems

In order for dynamic programming to be applicable, the problem must exhibit *optimal substructure*. This means that we can break the problem down into subproblems (much like divide and conquer) such that the subproblems can be recombined to form a solution to the original problem. In contrast with divide and conquer, the subproblems of a dynamic programming solution are repeated or overlapping, that is, they must be required many times (think computation of Fibonacci numbers). The easiest way to think about a dynamic programming problem is to try to break the problem up into a sequence of choices which lead us between subproblems. For example, in the coin change problem, our choices are the coins that we select. Every time we select a coin, our subproblem reduces in value by the dollar amount of the coin we just selected.

If we need to make $\$V$ and we choose to use a coin with value $\$x$, then we are now required to make change for $\$(V-x)$. The essence of dynamic programming is then to try every possible choice and take the best one, while memoising the answers to avoid repeated computation. Using this idea, the subproblems for coin change can be expressed as

$$\text{MinCoins[v]} = \{\text{The fewest coins required to make exactly \$v}\},$$

for all values of $v$ in $0 \leq v \leq V$. These subproblems exhibit optimal substructure since if the optimal solution for $\$V$ includes a coin of value $x$, then the remaining coins must necessarily be optimal for the value $\$(V-x)$.

### Deriving the recurrence

Now that we have our subproblems, we write a recurrence relation that expresses the optimal substructure and encompasses all of the possible choices we could make, taking the best one. If we use a coin of value $\$c_i$ when trying to make $\$v$, then we must recursively try to make $\$(v-c_i)$. The following recurrence tries all possible coins and selects the best option.

$$\text{MinCoins[v]} = \begin{cases} 0 & \text{if } v = 0, \\ \infty & \text{if } v < c[i] \text{ for all } i, \\ \min\limits_{\substack{1 \leq i \leq n \\ c[i] \leq v}} (1 + \text{MinCoins[v - c[i]]}) & \text{otherwise} \end{cases}$$

We include the base case MinCoins[0] = 0 since the recurrence must terminate, and it takes zero coins to make zero dollars. We also write the infeasible case (returning $\infty$) in case it is not possible to make some values, since there might not necessarily be a $1 coin.

### Implementing a solution

We can implement a top-down solution to coin change by implementing the recurrence relation above as a recursive function. Your implementation might look like the pseudocode shown in Algorithm 25. Note that we use memoisation to avoid computing a solution to a subproblem twice! Assume that the memo table is appropriately initialised to **null** before calling COIN_CHANGE.

**Algorithm 25** Top-down coin change

```
1:  function COIN_CHANGE(c[1..n], v)
2:      if v = 0 then return 0
3:      if memo[v] = null then
4:          min_coins = ∞
5:          for i = 1 to n do
6:              if c[i] ≤ v then
7:                  min_coins = min(min_coins, 1 + coin_change(v - c[i]))
8:              end if
9:          end for
10:         memo[v] = min_coins
11:     end if
12:     return memo[v]
13: end function
```

Since we solve $V+1$ subproblems and each one tries all $n$ coins, the time complexity of this solution is $O(nV)$. The space complexity of storing the solutions to $V$ subproblems is $O(V)$. Just as we did for Fibonacci numbers, we could also convert this into a bottom-up solution. Psuedocode for a bottom-up coin change algorithm is given in Algorithm 26.

**Algorithm 26** Bottom-up coin change

```
1:  function COIN_CHANGE(c[1..n], V)
2:      Set MinCoins[0..V] = ∞
3:      MinCoins[0] = 0
4:      for v = 1 to V do
5:          for i = 1 to n do
6:              if c[i] ≤ v then
7:                  MinCoins[v] = min(MinCoins[v], 1 + MinCoins[v - c[i]])
8:              end if
9:          end for
10:     end for
11:     return MinCoins[V]
12: end function
```

## Top-down vs. Bottom-up Dynamic Programming

Both styles of dynamic programming, top down and bottom up involve using a table to remember the solutions to previously computed subproblems. Their behaviour is quite different however. In the top-down approach, the memoisation table is filled on demand as the particular subproblems that are required are computed. In the bottom-up approach, we fill the solution table one problem at a time in an order which ensures that any dependent subproblems have already been computed before they are needed. The order in which we will the table in the bottom-up approach is the *reverse topological order* of the dependency graph of the subproblems (we will learn about topological orderings later in the unit.) Most of the time, figuring out the order in which the subproblems must be computed is simple, but in rare cases it might be more difficult.

The majority of the time, the two dynamic programming styles are equivalent and equally as good, but there are certain situations in which it may be preferable to favour one over the other. As eluded to above, one reason that the top-down approach might be preferable in some cases is that we do not need to know a-priori the order in which the subproblems need to be computed, as the recursion takes care of ensuring that subproblems are made available when required. The top-down approach also boasts the advantage that subproblems are only computed if they are actually required, while the bottom-up approach strictly computes the solution to every possible subproblem. If the solutions to only a small number of the possible subproblems are required, then the top-down approach will avoid computing the ones that are not needed.

On the contrary, the bottom-up approach avoids recursion altogether and hence should be faster if subproblems are frequently revisited since we drop the overhead on the program's call stack required to make the recursive calls. The bottom-up approach also allows us to more easily exploit the structure of specific dynamic programs in situations where we can improve the time and space complexity of the resulting program. We will see one such example, the space-saving trick in the next section, which allows us to reduce the space complexity of various dynamic programs, which is not possible with the top-down approach. The following table summarises the pros and cons of both approaches.

| **Pros: Top-down Approach** | **Pros: Bottom-up Approach** |
|---|---|
| 1. No need to know the topological ordering of the subproblem dependencies<br>2. Avoids computing the solution to subproblems that are not needed<br>3. More intuitive for programmers who like to think recursively | 1. Avoids recursion, which is typically slower than iteration<br>2. Allows for clever optimisations (e.g. space-saving trick in the next section)<br>3. Might be more intuitive for programmers who don't like recursion |

## Reconstructing Optimal Solutions to Optimisation Problems

When we solved the coin change problem, we left out something rather important. Although we computed the fewest number of coins required, we did not actually produce a list of those coins. We can extend our dynamic programming algorithm to also produce an optimal list of coins. In general, there are two ways to approach constructing an optimal solution.

### Method 1: Backtracking through the subproblems

The first way to reconstruct solutions to optimisation problems is to *backtrack* through the subproblems and figure out which choices were made that lead to the given solution. For example, in the coin change example given earlier, the fewest coins needed to make \$13 was three, so we could backtrack through the entries of the dynamic programming table over values of i = 1 to $n$ until we found a coin $c_i$ such that MinCoins[13 - $c_i$] = 2. When we find such a coin, the optimal substructure of the problem tells us that this coin is optimal. We then subtract $c_i$ from 13 and repeat until we reach $V = 0$ at which point we know we have constructed the entire solution. An example implementation using the bottom-up approach is shown in Algorithm 27.

**Algorithm 27** Coin change solution reconstruction using backtracking

```
1:  function GET_COINS(c[1..n], V, MinCoins[0..V])
2:      if MinCoins[V] = ∞ then return error
3:      Set coins = empty list
4:      while V > 0 do
5:          for i = 1 to n do
6:              if c[i] ≤ V and MinCoins[V] = 1 + MinCoins[V - c[i]] then      // c[i] is optimal
7:                  coins.append(c[i])
8:                  V = V - c[i]
9:              end if
10:         end for
11:     end while
12:     return coins
13: end function
```

### Method 2: Using a decision table

The second approach often used for reconstructing solutions is to keep a second table in addition to the memoisation or bottom-up dynamic programming table which is used to remember the optimal decisions that were made by each subproblem. Once the optimal value is found, the solution can then be reconstructed by looking up the choices that were made in this table. An implementation of coin change using this approach is shown in Algorithm 28. In this implementation, we store an array OptCoin in addition to the MinCoins array, which remembers for each value of $v$, a coin that would lead to the optimal solution.

**Algorithm 28** Bottom-up coin change with solution reconstruction using decision table

```
1:  function COIN_CHANGE(c[1..n], V)
2:      Set MinCoins[0..V] = ∞
3:      Set OptCoin[0..V] = null
4:      MinCoins[0] = 0
5:      for v = 1 to V do
6:          for i = 1 to n do
7:              if c[i] ≤ v then
8:                  if 1 + MinCoins[v - c[i]] < MinCoins[v] then
9:                      MinCoins[v] = 1 + MinCoins[v - c[i]]
10:                     OptCoin[v] = c[i]        // Remember the best coin
11:                 end if
12:             end if
13:         end for
14:     end for
15:     return MinCoins[v]
16: end function
17:
18: function GET_COINS(c[1..n], V, MinCoins[0..V], OptCoin[0..V])
19:     if MinCoins[V] = ∞ then return error
20:     Set coins = empty list
21:     while V > 0 do
22:         coins.append(OptCoin[V])        // Take the best coin
23:         V = V - OptCoin[V]
24:     end while
25:     return coins
26: end function
```

Both approaches are very similar. The first is advantaged by the fact that it uses less memory, since a second table is not required to remember the optimal coins. It should also usually be faster as a consequence. The second approach however is simpler to understand, and also allows us to do some more advanced optimisations that involve dynamically adjusting the search space for a particular subproblem based on the optimal choices of previous subproblems.

# Chapter 6

# Dynamic Programming: Part II

Now that we have been introduced to the powerful dynamic programming paradigm, we will take a look at a few more classic problems that can be solved using it.

**Summary: Dynamic Programming: Part II**

In this chapter, we cover:

- More dynamic programming!
- The unbounded knapsack problem
- The 0-1 knapsack problem
- Optimal matrix multiplication (**Not examinable in Semester Two, 2018**)
- The edit distance problem
- The space-saving trick

**Recommended Resources: Dynamic Programming**

- CLRS, Introduction to Algorithms, Chapter 15
- Weiss, Data Structures and Algorithm Analysis, Section 10.3
- Halim, Competitive Programming 3, Section 3.5
- `https://youtu.be/ocZMDMZwhCY` - MIT 6.006 lecture on DP: Part III
- `http://users.monash.edu/~lloyd/tildeAlgDS/Dynamic/`
- `http://users.monash.edu/~lloyd/tildeAlgDS/Dynamic/Edit/`

## The Unbounded Knapsack Problem

Suppose you find yourself in a room full of $n$ heavy but valuable kinds of items! You have with you a backpack that you can use to carry up to $C$ kilograms of items. You have figured out for each kind of item $i$ how valuable it is $v_i$ and how much it weighs $w_i$. Which items should you take in order to maximise the total value in your backpack? We can consider two different versions of this problem. In the first one, we can take as many of each kind of item as we want.

This is called the *unbounded* knapsack problem. In the second version, which we will cover next, we can only take one of each kind.

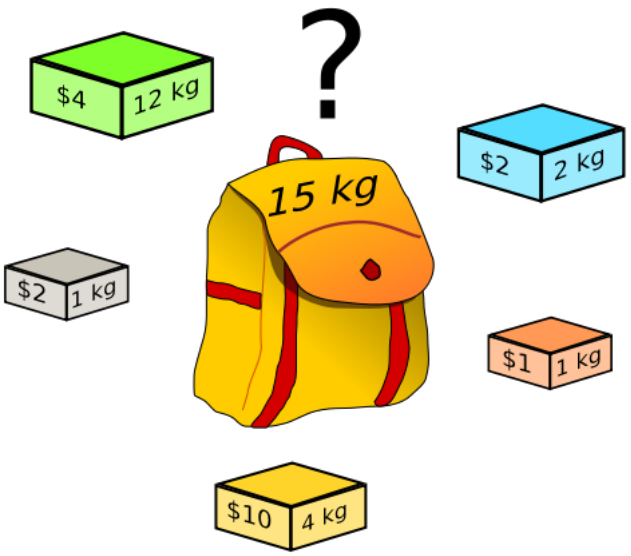



Figure 6.1: An example instance of a knapsack problem. The optimal solution is to take all but the green box for a total value of $15. Image taken from Wikimedia Commons[1].

We can solve the unbounded knapsack problem using dynamic programming. Let's walk through the process.

## Identifying the optimal subproblems

The unbounded knapsack problem is actually rather similar to the coin change problem. In coin change, we were selecting coins such that made exactly $\$V$ using the fewest coins possible. Now we are selecting items that weigh at most $C$kg that have the highest value possible. Both problems have a capacity constraint, although unlike coin change, for the knapsack problem it is not required that we leave no empty space. Both of them are also optimising an objective based on the items selected, except that for coin change we are minimising and for knapsack we are maximising. The decisions that we can make in the knapsack problem are the items that we select, analogous to the coins that we select for the coin change problem.

Suppose that we are trying to fill a bag with capacity $C$kg. If we choose an item with weight $x$kg, we are then required to fill the remaining $(C-x)$kg of space with the most valuable items. This substructure is optimal since we always want to use the remaining $(C-x)$kg optimally. This suggests that our subproblems should be the following:

$$\text{MaxValue}[c] = \{\text{The maximum value that we can fit in a capacity of } c\}$$

for values of $c$ such that $0 \leq c \leq C$.

[1] Taken from `https://en.wikipedia.org/wiki/File:Knapsack.svg` by Dake. Shared under a creative commons licence.

### Deriving a recurrence

Using the substructure that we derived above, we can write a recurrence for the unbounded knapsack problem like so:

$$\text{MaxValue}[c] = \begin{cases} 0 & \text{if } c < w_i \text{for all } i, \\ \max\limits_{\substack{1 \le i \le n \\ w_i \le c}} (v_i + \text{MaxValue}[c - w_i]) & \text{otherwise.} \end{cases}$$

Notice that we do not need an infeasible case like we did for coin change since we are not requiring that the knapsack be completely full.

### Implementation of the unbounded knapsack problem

A bottom-up implementation of the unbounded knapsack dynamic program is shown in Algorithm 29. Note how extremely similar it ends up being to the bottom-up solution for coin change.

**Algorithm 29** Bottom-up unbounded knapsack

```
1:  function UNBOUNDED_KNAPSACK(v[1..n], w[1..n], C)
2:      Set MaxValue[0..C] = 0
3:      for c = 1 to C do
4:          for i = 1 to n do
5:              if w[i] ≤ c then
6:                  MaxValue[c] = max(MaxValue[c], v[i] + MaxValue[c - w[i]])
7:              end if
8:          end for
9:      end for
10:     return MaxValue[C]
11: end function
```

## The 0-1 Knapsack Problem

We now consider a variant of the knapsack problem in which we are only allowed to take one of each kind of item. This problem is known in general as the 0-1 knapsack problem (0-1 because we can either take 0 of the item or 1 of it) One method to solve the knapsack problem is to simply try all possibilities and see which one is the best feasible solution. If we have $n$ items to choose from, then we would have to try all possible subsets of $n$ items. The total number of subsets of a set of $n$ items is $2^n$, so trying all of them would lead to an exponential time complexity algorithm! We can use dynamic programming to derive a much more efficient and elegant solution to the knapsack problem.

## Identifying the optimal subproblems

Consider an instance of the knapsack problem, for example, the one shown in Figure 6.1. The optimal solution for the five items shown given a backpack that carry a total weight of 15kg is to take the blue, silver, yellow and orange items for a total of $15 value. The optimal substructure for 0-1 Knapsack is almost identical to that of the unbounded version, but we need to account for the fact that an item can not be used twice.

Suppose we try the blue item. Since it takes up precisely 2kg of the 15kg backpack, there is 13kg of space left for other items. We are then left with solving the subproblem of finding the most value that we can accrue using 13kg of spacing **using the remaining items**. This is the optimal substructure of the 0-1 knapsack problem. Note the emphasis highlighting the difference compared to the unbounded version. In the 0-1 case, we need to never consider an item again if it has already been used. One way to do this would be to keep track of the subset of items that have been used so far, but this does not improve on the naive solution since we would need to account for $2^n$ different subsets, which is far too large for moderate values of $n$. Instead, the key observation to make is that the order in which we consider items is completely irrelevant since taking the 2kg item followed by the 4kg item is the same as taking the 4kg item followed by taking the 2kg item. Therefore instead of keeping track of all subsets, we will just remember that we have taken some items from the first $i$ of them, for all values of $i$ from $1 \leq i \leq n$.

$$\text{MaxValue}[i, c] = \{\text{The maximum value that we can fit in a capacity of } c \text{ using items 1 to } i\}$$

for all $0 \leq c \leq C$ and $0 \leq i \leq n$. This way, if we choose to take item $i$, then we know that we can subsequently only consider items 1 to $i-1$. Note that by $i = 0$, we denote the empty set of items to give us a simple base case.

## Deriving a recurrence

Consider an instance of the knapsack problem consisting of $n$ items of weight $w_i$ and value $v_i$ for $1 \leq i \leq n$ and a backpack of capacity $C$ kg. Since we are avoiding duplicate items, we should not try using every item in the backpack, but rather, in a subproblem considering items 1 to $i$, we should simply try taking item $i$ or not taking item $i$. This gives us two options, both of which lead to recursively trying to fill the knapsack with the remaining items 1 to $i-1$.

$$\text{MaxValue}[i, c] = \begin{cases} 0 & \text{if } i = 0, \\ \text{MaxValue}[i-1, c] & \text{if } w_i > c, \\ \max(\text{MaxValue}[i-1, c], v_i + \text{MaxValue}[i-1, c-w_i]) & \text{otherwise.} \end{cases}$$

In the second case of the recurrence, we account for the fact that item $i$ may not fit in the knapsack, in which case there is no decision to make, we simply can not take that item and should consider the remaining $i-1$ items.

## Implementation of the 0-1 knapsack problem

Here is a bottom-up implementation of the dynamic programming algorithm corresponding to the recurrence derived above. Each row of the recurrence depends only on the previous row, so

we will solve the subproblems in row order. See Algorithm 30. Since there are $n \times C$ subproblems and solving each one requires looking at no more than two previous subproblems, the time and space complexities of this dynamic programming algorithm are $O(nC)$.

**Algorithm 30** Bottom-up 0-1 knapsack

```
1:  function KNAPSACK(w[1..n], v[1..n], C)
2:      Set MaxValue[0..n][0..C] = 0
3:      for i = 1 to n do
4:          for c = 1 to C do
5:              if w[i] ≤ c then
6:                  MaxValue[i][c] = max(MaxValue[i-1][c], v[i] + MaxValue[i-1][c - w[i]])
7:              else
8:                  MaxValue[i][c] = MaxValue[i-1][c]
9:              end if
10:         end for
11:     end for
12:     return MaxValue[n][C]
13: end function
```

## The Edit Distance Problem

The edit distance problem is a way to formally classify how similar or dissimilar two strings of text are. For example, the words "computer" and "commuter" are similar, as we can change one into the other by just modifying one letter, 'p' to 'm.' The words "sport" and "sort" are similar, as one can be changed into the other by deleting one letter from the first (or equivalently, inserting a new letter into the second).

This notion of the number of "edits" required to transform one string into another form the basis of the edit distance metric. A single edit operations consists of one of the following three operations:

1. Insert a new symbol anywhere in the string
2. Delete one of the symbols from the string
3. Replace one of the symbols in the string with any other symbol

**Definition: Edit Distance**

The edit distance between two strings is the minimum number of edit operations required to convert one of the strings into the other.

We can also define an optimal alignment of two strings which shows where the optimal number of insertions, deletions and substitutions occur. An optimal alignment for "computer" and "commuter" would be

| c | o | m | **p** | u | t | e | r |
|---|---|---|---|---|---|---|---|
| c | o | m | **m** | u | t | e | r |
| | | | * | | | | |

which contains one edit operation (substitute 'p' for 'm.') An optimal alignment for the words "kitten" and "sitting" is given by

| **k** | i | t | t | **e** | n | - |
|---|---|---|---|---|---|---|
| **s** | i | t | t | **i** | n | **g** |
| * | | | | * | | * |

which contains two substitutions and one insertion, so the edit distance between them is 3.

## Identifying the optimal subproblems

Consider the problem of finding an optimal alignment for the strings "ACAATCC" and "AGCATCG." Considering just the final column of the alignment, we have three choices:

| C | | C | | - |
|---|---|---|---|---|
| G | or | - | or | G |
| * | | * | | * |

The first choice corresponds to substituting the last 'C' for 'G.' The second choice corresponds to deleting the last 'C,' and the third choice corresponds to inserting the character 'G' at the end of the string. Once we have made a choice of one of these three options, we are then left to find an optimal alignment of all of the remaining characters. In other words, the optimal alignment of "ACAATCC" and "AGCATCG" is one of:

$$\text{OPTIMAL\_ALIGNMENT}(\text{"ACAATC"}, \text{"AGCATC"}) + \begin{bmatrix} \texttt{C} \\ \texttt{G} \\ * \end{bmatrix}$$

$$\text{OPTIMAL\_ALIGNMENT}(\text{"ACAATC"}, \text{"AGCATCG"}) + \begin{bmatrix} \texttt{C} \\ \texttt{-} \\ * \end{bmatrix}$$

$$\text{OPTIMAL\_ALIGNMENT}(\text{"ACAATCC"}, \text{"AGCATC"}) + \begin{bmatrix} \texttt{-} \\ \texttt{G} \\ * \end{bmatrix}$$

The alignment of the remaining prefixes must be optimal because if it were not, we could substitute it for a more optimal one and achieve a better overall alignment. Let us therefore define our subproblems as follows:

$$\text{Dist}[i, j] = \{\text{The edit distance between the prefixes } S_1[1..\text{i}] \text{ and } S_2[\text{i..j}]\}$$

for $0 \leq i \leq n$, $0 \leq j \leq m$.

## Deriving a recurrence

Using the optimal subproblems observed above, we can derive a recurrence for the edit distance between two strings $S_1[1..n]$ and $S_2[1..m]$ like so. Consider the computation of the subproblem $\text{Dist}[i, j]$, where $i, j > 0$. We have three choices:

1. Align $S_1[i]$ with $S_2[j]$, which has a cost of zero if $S_1[i] = S_2[j]$, or one otherwise.
2. Delete the character $S_1[i]$, which has a cost of one
3. Insert the character $S_2[j]$, which has a cost of one

If we choose to align $S_1[i]$ with $S_2[j]$, then the subproblem that remains to be solved is to align the remaining prefixes i.e. to minimise $\text{Dist}[i-1, j-1]$. If we delete the character $S_1[i]$, then we need to align the remaining prefix of $S_1$ with $S_2$, i.e. we are interested in minimising the subproblem $\text{Dist}[i-1, j]$. Finally, if we chose to insert the character $S_2[j]$, then we are left to align the remaining prefix of $S_2$ with $S_1$, i.e. we want to optimise the subproblem $\text{Dist}[i, j-1]$. Trying all three possibilities and selecting the best one leads to the following general recurrence for $\text{Dist}[i, j]$.

$$\text{Dist}[i,j] = \begin{cases} i & \text{if } j = 0, \\ j & \text{if } i = 0, \\ \min \begin{cases} \text{Dist}[i-1, j-1] + 1_{S_1[i] \neq S_2[j]} \\ \text{Dist}[i-1, j] + 1 \\ \text{Dist}[i, j-1] + 1 \end{cases} & \text{otherwise} \end{cases}$$

We have used the notation $1_{S_1[i] \neq S_2[j]}$ to denote an indicator variable for $S_1[i] \neq S_2[j]$. In other words, it equals one if $S_1[i] \neq S_2[j]$, or zero otherwise. The base cases should be easy to understand. If one of the two strings is empty, then an optimal alignment simply consists of inserting all of the characters of the other string.

## Implementation of edit distance

A bottom-up implementation of the dynamic programming solution for the edit distance problem is shown in Algorithm 31. We note that the order in which we must compute the subproblems corresponds to prefixes of increasing length since each subproblem depends only on the subproblems of length one shorter. There are a total of $n \times m$ subproblems, and computing the solution to each one requires us to look back at just three previous ones, hence the time and space complexity of the edit distance dynamic programming algorithm is $O(nm)$.

## Constructing an optimal alignment

In order to construct the alignment for the strings $S_1$ and $S_2$, we need to backtrack through the dynamic programming subproblems from $\text{Dist}[n, m]$ to $\text{Dist}[0, 0]$, examining the choices that were made along the way. The following function shown in Algorithm 32 takes the filled dynamic programming table $\text{Dist}[0..n][0..m]$ and produces the alignment. Note that we build the alignment in reverse since we backtrack from the ends of the strings.

**Algorithm 31** Bottom-up edit distance

```
1:  function EDIT_DISTANCE(S1[1..n], S2[1..m])
2:      Set Dist[0..n][0..m] = 0
3:      Set Dist[1..n][0] = 1..n
4:      Set Dist[0][1..m] = 1..m
5:      for i = 1 to n do
6:          for j = 1 to m do
7:              if S1[i] = S2[j] then
8:                  Dist[i][j] = Dist[i-1][j-1]
9:              else
10:                 Dist[i][j] = min(Dist[i-1][j-1], Dist[i-1][j], Dist[i][j-1]) + 1
11:             end if
12:         end for
13:     end for
14:     return Dist[n][m]
15: end function
```

**Algorithm 32** Optimal sequence alignment

```
1:  function ALIGNMENT(S1[1..n], S2[1..m], Dist[0..n][0..m])
2:      Set A1 = "", A2 = ""
3:      Set i = n, j = m
4:      while i+j > 0 do
5:          if i = 0 then
6:              A1 += "-"
7:              A2 += S2[j]
8:              j = j - 1
9:          else if j = 0 then
10:             A1 += S1[i]
11:             A2 += "-"
12:             i = i - 1
13:         else
14:             Set best = min(Dist[i-1][j-1], Dist[i][j-1], Dist[i-1][j])
15:             if S1[i] = S2[j] or Dist[i-1][j-1] = best then      // Substitution
16:                 A1 += S1[i]
17:                 A2 += S2[j]
18:                 i = i - 1
19:                 j = j - 1
20:             else if Dist[i-1][j] = best then      // Deletion from S1
21:                 A1 += S1[i]
22:                 A2 += "-"
23:                 i = i - 1
24:             else      // Insertion into S1
25:                 A1 += "-"
26:                 A2 += S2[j]
27:                 j = j - 1
28:             end if
29:         end if
30:     end while
31:     return reverse(A1), reverse(A2)
32: end function
```

## Matrix Multiplication (Not examinable in Semester Two, 2018)

Recall the problem of multiplying two matrices $A$ and $B$. If $A$ is an $n \times m$ matrix and $B$ is an $m \times o$ matrix, then their product will be an $n \times o$ matrix.

$$\underbrace{\begin{bmatrix} \\ A \\ \\ \end{bmatrix}}_{n \times m} \times \underbrace{\begin{bmatrix} \\ B \\ \\ \end{bmatrix}}_{m \times o} = \underbrace{\begin{bmatrix} \\ A \times B \\ \\ \end{bmatrix}}_{n \times o}$$

In general, the amount of work required to multiply an $n \times m$ matrix and an $m \times o$ matrix is $n \times m \times o$ scalar multiplications. Consider now the problem of multiplying a sequence of matrices of differing sizes. For example, suppose we want to compute the product of a $4 \times 2$, a $2 \times 5$ and a $5 \times 3$ matrix.

$$\underbrace{\begin{bmatrix} \\ A \\ \end{bmatrix}}_{4 \times 2} \times \underbrace{\begin{bmatrix} \\ B \\ \end{bmatrix}}_{2 \times 5} \times \underbrace{\begin{bmatrix} \\ C \\ \\ \end{bmatrix}}_{5 \times 3}$$

There are several ways that we could compute this product, owing to the fact that matrix multiplication is associative. This means that we can bracket the product in any way we want and we will still obtain the same answer. We can compute this product in either the order $(A \times B) \times C$ or $A \times (B \times C)$. Surprisingly, the order that choose to do the multiplications actually has a substantial effect on the amount of computational time required. If we choose the first order $(A \times B) \times C$, then we perform $(4 \times 2 \times 5) + (4 \times 5 \times 3) = 100$ scalar multiplications to obtain the answer. If we use the second order $A \times (B \times C)$, then we only perform $(2 \times 5 \times 3) + (4 \times 2 \times 3) = 54$ scalar multiplications. That's almost half the amount of work! The general optimal matrix multiplication problem is the problem of deciding for a sequence of $n$ matrices, the best way to multiply them to minimise the number of scalar multiplications required.

For a sequence of four matrices, there are five different ways to parenthesise them as follows: $A \times ((B \times C) \times D)$, $A \times (B \times (C \times D))$, $(A \times B) \times (C \times D)$, $(((A \times B) \times C) \times D)$ and $(A \times (B \times C)) \times D$. In general, the number of ways to parenthesise a sequence of $n$ matrices is exponential in $n$ (it is related to the famous Catalan number sequence), so trying all of them would be way too slow. Dynamic programming can be used to find a fast solution to the optimal matrix multiplication problem.

### Identifying the optimal subproblems

Consider a sequence of $n$ matrices $A_1, A_2, A_3, A_4, ...A_n$ to be multiplied (assume that they are of valid dimensions to be multiplied.) Think about the final multiplication that happens in the

sequence. This multiplication must be the product of two matrices

$$\underbrace{(A_1 \times A_2 ... \times A_k)}_{\substack{\text{Result of multiplying} \\ \text{matrices 1 to } k}} \times \underbrace{(A_{k+1} \times A_{k+2} \times ... \times A_n)}_{\substack{\text{Result of multiplying} \\ \text{matrices } k+1 \text{ to } n}},$$

where $(A_1 \times A_2 ... \times A_k)$ and $(A_{k+1} \times A_{k+2} \times ... \times A_n)$ were multiplied earlier. If this is the optimal order in which to multiply the matrices, then the two subproblems of multiplying $(A_1 \times A_2 ... \times A_k)$ and $(A_{k+1} \times A_{k+2} \times ... \times A_n)$ must also be multiplied in optimal order. If they were not, we could substitute them for a better order and obtain a better solution. This is the optimal substructure for the optimal matrix multiplication problem.

The dynamic programming solution for the optimal matrix multiplication problem therefore involves trying every possible "split point" $k$ at which to perform the final multiplication. The problem is then recursively solved by asking for the optimal order in which to multiply matrices 1 to $k$ and the remaining matrices $k+1$ to $n$. Our subproblems should therefore be:

$$\text{DP}[i, j] = \{\text{The minimum number of multiplications required to multiply } (A_i, A_{i+1}, ...A_j)\}$$

for all $1 \leq i \leq j \leq n$.

## Deriving a recurrence

Let us denote the number of columns in the matrices $A_1, A_2, ...A_n$ by the sequence $c_1, c_2, ..., c_n$. Recalling that two adjacent matrices can only be multiplied if the number of columns of the first is the same as the number of rows of the second, we know that if the sequence of matrices $(A_i)$ is valid, that the number of rows in $A_2, ...A_n$ must be $c_1, ...c_{n-1}$. For completeness, we will further denote the number of rows of $A_1$ as $c_0$. A base case for our problems is easy to identify. It takes zero multiplications to multiply a sequence of just one matrix. So $\text{DP}[i, i] = 0$ for all $i$.

For the general case, to find the optimal number of multiplications for the sequence $A_i, ...A_j$ where $i < j$, we must try every possible "split point" and recurse. If we perform the split after matrix $k$, where $i \leq k < j$, then the total number of required multiplications is $\text{DP}[i, k] + \text{DP}[k+1, j]$ plus the number of multiplications required to multiply $(A_i \times ... \times A_k)$ and $(A_{k+1} \times ... \times A_j)$. The matrix $(A_i \times ... \times A_k)$ has exactly $c_{i-1}$ rows and $c_k$ columns, and the matrix $(A_i \times ... \times A_k)$ and $(A_{k+1} \times ... \times A_j)$ has exactly $c_k$ rows and $c_j$ columns. Hence the number of scalar multiplications required to multiply them is $c_{i-1} \times c_k \times c_j$. Therefore the total number of required multiplications to multiply matrices $i$ to $j$ if we split after matrix $k$ is given by

$$\text{DP}[i, j] = \text{DP}[i, k] + \text{DP}[k+1, j] + c_{i-1} \times c_k \times c_j.$$

Combining everything together and trying all possible split points, we end up with the recurrence

$$\text{DP}[i, j] = \begin{cases} 0 & \text{if } i = j \\ \min\limits_{i \leq k < j} (\text{DP}[i, k] + \text{DP}[k+1, j] + c_{i-1} c_k c_j) & \text{if } i < j. \end{cases}$$

for $i \leq j \leq n$. Note that we do not care about defining $\text{DP}[i, j]$ for $j > i$ since it does not make sense to have reversed intervals. With this recurrence, the answer to the entire problem is $\text{DP}[1, n]$, the optimal number of scalar multiplications required to multiply the entire sequence $A_1 \times ... \times A_n$.

## Implementation of optimal matrix multiplication

Let's write a bottom-up solution to optimal matrix multiplication. First, we must consider the order in which the subproblems depend on each-other. For each subproblem DP$[i, j]$, we need to have already computed the values of DP$[i, k]$ and DP$[k+1, j]$ for all $i \leq k < j$. This means that it would be incorrect to simply loop over all $1 \leq i \leq j$ and $1 \leq j \leq n$ as we might be naturally inclined to. The essential observation is that the subproblems depend on subproblems consisting of a shorter sequence of matrices. A valid order in which to compute the solutions is therefore in order of length, i.e. we compute the answer for all contiguous subsequences of 2 matrices, then all contiguous subsequences of 3 matrices and so on. The algorithm is depicted in Algorithm 33.

**Algorithm 33** Optimal matrix multiplication

```
1:  function MATRIX_ORDER(c[0..n])
2:      Set DP[1..n][1..n] = 0
3:      for length = 2 to n do
4:          for i = 1 to n - length + 1 do
5:              Set j = i + length - 1
6:              Set best = ∞
7:              for k = i to j - 1 do
8:                  best = min(best, DP[i][k] + DP[k+1][j] + c[i-1] × c[k] × c[j])
9:              end for
10:             DP[i][j] = best
11:         end for
12:     end for
13:     return DP[1][n]
14: end function
```

Since there are $n^2/2$ subproblems and the computation of each subproblem $i, j$ requires looping over $j-i$ previous subproblems, the time complexity of the dynamic programming solution for optimal matrix multiplication is

$$\begin{aligned}
\sum_{i=1}^{n}\sum_{j=i+1}^{n}(j-i) &= \sum_{i=1}^{n}\left(\sum_{j=i+1}^{n} j - \sum_{j=i+1}^{n} i\right), \\
&= \sum_{i=1}^{n}\sum_{j=i+1}^{n} j - \sum_{i=1}^{n}(n-i)i, \\
&= \sum_{i=1}^{n}\left(\frac{n(n+1)}{2} - \frac{i(i+1)}{2}\right) - n\sum_{i=1}^{n} i + \sum_{i=1}^{n} i^2, \\
&= \frac{n^2(n+1)}{2} - \frac{1}{2}\left(\sum_{i=1}^{n} i^2 + \sum_{i=1}^{n} i\right) - \frac{n^2(n+1)}{2} + \sum_{i=1}^{n} i^2, \\
&= \frac{n(n+1)}{4} + \frac{1}{2}\sum_{i=1}^{n} i^2.
\end{aligned}$$

Finally, using the sum of squares formula, $\sum_{i=1}^{n} i^2 = \frac{n(n+1)(2n+1)}{12}$, we obtain

$$\begin{aligned}\sum_{i=1}^{n}\sum_{j=i+1}^{n}(j-i) &= \frac{n(n+1)}{4} + \frac{1}{2}\sum_{i=1}^{n} i^2 \\ &= \frac{n(n+1)}{4} + \frac{n(n+1)(2n+1)}{12},\end{aligned}$$

which is $O(n^3)$. Since we have $O(n^2)$ subproblems, the space complexity is $O(n^2)$.

## The Space-Saving Trick

You may have noticed that the recurrences for the edit distance problem and the 0-1 knapsack problem both had a very interesting property. Despite having a 2 dimensional table of subproblems, each subproblem only ever depended on subproblems from the previous row in order to compute it's optimal solution. Because of this, we do not need to keep the entire table in memory all at once. It is enough to simply store two rows of the table at a time, and re-use the same memory for every second row of subproblems that we compute. This reduces the space complexity of the edit distance and knapsack problems to $O(\min(n,m))$ and $O(C)$ respectively. Of course, we have to remember that if we employ the space-saving trick, we can no longer backtrack through the subproblems to construct the optimal solution.

# Chapter 7

# Hashing and Hashtables

Storing and retrieving data is one of the most common scenarios in which we employ advanced data structures. We will first look at arguably one of the most well-known data structures in computer science, hashing. Hashing aims to solve the "dictionary" problem, where we need to store an search for items associated with keys. Using hashing, we can usually support these operations in just $O(1)$ expected time! We will briefly revise the basic hashing schemes that you should be familiar with, hashing with chaining and hashing with open addressing (probing). Then we will cover a selection of good hash functions for random integer keys and string keys, and briefly discuss the roll of randomness in produces good hashes. We will then discuss a more advanced hashtable strategy, cuckoo hashing.

**Summary: Hashing and Hashtables**

In this chapter, we cover:

- The dictionary problem and hashtables (Revision)
- Collision resolution strategies (Revision)
- Good hash functions for integers
- Hash functions for strings
- Universal hashing (**Not examinable in Semester Two, 2018**)
- Cuckoo hashing

**Recommended Resources: Hashing and Hashtables**

- CLRS, Introduction to Algorithms, Chapter 11
- Weiss, Data Structures and Algorithm Analysis, Chapter 5
- Knuth, The Art of Computer Programming, Volume 3, Section 6.4
- `https://visualgo.net/en/hashtable` - Visualisation of Hashtables
- `https://youtu.be/0M_kIqhwbFo` - MIT 6.006 lecture on hashing
- `https://youtu.be/rvdJDijO2Ro` - MIT 6.006 lecture on open address hashing
- `http://users.monash.edu/~lloyd/tildeAlgDS/Table/`

# The Dictionary Problem

The dictionary problem is arguably the most frequently applicable problem in computer science. The dictionary abstract data type (ADT) supports the following operations:

1. INSERT(item): insert an item with a given key into the dictionary
2. DELETE(item): delete an item with a given key from the dictionary
3. LOOKUP(key): find the item with the given key if it exists

We assume that all items have unique keys, and that all keys come from a universe $\mathscr{U}$, typically integers $\{0,1,...,u-1\}$. Non-integer keys should be converted to integers. We will see in the next chapter that this problem can be solved using balanced binary search trees in $O(\log(n))$ time per operation, but we want to do better than this. The goal of hashtables is to solve the dictionary problem in just $O(1)$ expected time per operation.

# Hashtables (Revision)

## Direct addressing

The simplest way to solve the dictionary problem is with *direct addressing*. A direct address table is a table of size $|\mathscr{U}|$, where we insert key $k$ into slot $k$ of the table. This allows for worst-case $O(1)$ insertion, deletion, and lookup! Of course, this scheme is only practical when the universe $\mathscr{U}$ is small, otherwise we will not have enough memory to store a direct address table.

## Hashing

The solution to the prohibitive memory usage of direct addressing is to employ *hashing*. We reduce the universe $\mathscr{U}$ down to a size that we can manage, say integers $\{0,1,...,m-1\}$ and use a *hash function*

$$h : \mathscr{U} \to \{0,1,...,m-1\},$$

to map keys onto the reduced universe. Items are then stored in a table of size $m$, with key $k$ being stored at position $h(k)$. This allows us to control the memory usage, but introduces a new problem. Since it is likely that $m \ll |\mathscr{U}|$, it will be the case that there are distinct pairs of keys $k_i, k_j$ such that $h(k_i) = h(k_j)$, i.e. they will map to the same value. We call such a pair of keys a *collision*. We will explore several strategies for resolving collisions. First, we revise chaining and open addressing. Later, we will explore an entirely different strategy, Cuckoo hashing.

## Chaining

Collision resolution via chaining involves maintaining a linked list at every position $0,1,...,m-1$ in the table and inserting all elements with $h(k) = i$ into the linked list at position $i$. If we assume that every key is equally likely to be hashed to any slot in the table (unachievable in practice!) then the expected number of items in each chain is $n/m$, where $n$ is the number of items in the

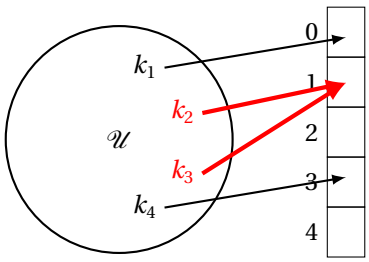



Figure 7.1: A hashtable with collisions

hashtable. We call the quantity $\alpha = n/m$ the *load factor*. Given that the expected chain length is $\alpha$, the expected time complexity for chaining is therefore $O(1+\alpha)$ per operation. If we keep $m \geq n$, which implies $\alpha \leq 1$, this yields expected $O(1)$ performance per operation!

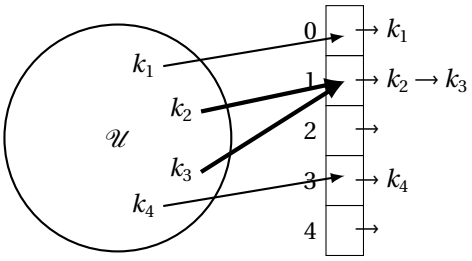



Figure 7.2: Hashing with chaining

## Open Addressing (Probing)

Open addressing involves storing all of the items in the table directly. This means that we strictly need $m \geq n$, i.e. $\alpha \leq 1$. In open addressing, whenever a collision occurs, we seek an alternate location to place the key. We do so by *probing*. We adjust our hash function so that instead of suggesting a single location, it suggests a sequence of locations for us to try.

$$h(k,i) : \mathscr{U} \times \mathbb{N} \rightarrow \{0,1,...,m-1\}$$

Deletion must be done with caution when using open addressing. Simply removing an item from the table may make other items unreachable if they were placed there via probing. To account for this, we should mark deleted slots with a flag that insertion is free to ignore and overwrite, but lookup should interpret as an occupied slot.

If we assume that for every key, each of the possible $m!$ probe sequences are equally likely and that keys are randomly distributed in the table (also not achievable in practice, but easy to analyse), then the expected time complexity per operation using open addressing is $O\left(\frac{1}{1-\alpha}\right)$ since we have probability at least $\frac{m-n}{m}$ of finding an empty slot each probe, which implies an expected number of trials at most equal to

$$\frac{1}{\frac{m-n}{m}} = \frac{m}{m-n} = \frac{\frac{m}{m}}{\frac{m}{m} - \frac{n}{m}} = \frac{1}{1-\alpha}.$$

e.g. if $\alpha = 0.5$, we expect at most two probes, for $\alpha = 0.75$, four probes, etc. Keeping $\alpha$ below any fixed constant therefore implies that we can perform operations in expected $O(1)$ time. In practice, this means that we must increase the size of the table and select a new hash function whenever the load factor exceeds this selected threshold. Common thresholds used are 0.25, 0.5, 2/3, and 0.75 depending on the probing method used.

We will look at three probing strategies that are commonly employed.

#### Linear Probing

In linear probing, we probe adjacent locations in the table until we find an empty slot:

$$h(k,i) = (h'(k) + i) \mod m,$$

where $h'(k)$ is the original hash function. In theory, linear probing performs quite poorly since it is quite susceptible to *primary clustering*. If many keys end up around the same location, then it only further increases the probability that even more keys end up around that location. However in practice, linear probing is incredibly efficient due to cache locality.

#### Quadratic Probing

In quadratic probing, we follow the probe sequence:

$$h(k,i) = (h'(k) + c_1 i + c_2 i^2) \mod m,$$

where $h'(k)$ is the original hash function and $c_1$ and $c_2$ are chosen constants. Quadratic probing avoids the problem of primary clustering since keys jump further away, but we are still susceptible to *secondary clustering*, keys with the same hash values will always probe the same elements.

#### Double Hashing

Double hashing aims to avoid the problem of secondary clustering. In double hashing, we use a second hash function to determine the distance between probed elements.

$$h(k,i) = (h_1(k) + i\,h_2(k)) \mod m,$$

where $h_1(k)$ is the original hash function, and $h_2(k)$ is the secondary hash function. Although it eliminates secondary clustering, double hashing is sometimes less efficient in practice since two hash functions have to be computed

## What is a Good Hash Function?

Good hash functions are those which minimise the probability of collisions occurring. This is very easy to say, but very difficult, and sometimes impossible to achieve in practice. Assuming that the keys to be hashed are uniformly distributed implies that an ideal hash function maps

keys uniformly onto the range of potential hash values. For example, to hash keys which are floating point values in the range $0 \leq k \leq 1$, a hash function that maps onto the integers 0 to $m-1$ which satisfies this ideal is

$$h(k) = \lfloor km \rfloor$$

While this might be ideal under the assumption that the keys $k$ are uniformly distributed in $0 \leq k \leq 1$, this is a terrible hash function if it turns out that 99% of the keys $k$ turn out in practice to be very close together, as this hash function maps keys that are very close to the same hash value. In this scenario, an ideal hash function would be one that maps keys that are very close together to hash values that are very far apart.

What this really means is that unfortunately, it is not possible in general to design a hash function that is perfect for all situations. In fact in theory, the ideal hash function is actually the totally random hash function! A totally random hash function would map each potential input key to each potential slot in the hashtable with equal probability uniformly at random. Unfortunately, implementing a totally random hash function would use a prohibitive amount of time and memory to compute, since we would need to store a hash value for every possible input key in advance.

In the following sections, we will study some hash functions which are good under the assumption that the input keys are random. In practice, this is a bad assumption, since real-world data usually has biases! To account for this, we often introduce randomness into our hash functions, which we discuss later when we meet universal hashing.

## How likely are collisions?

Although collisions might seem rare, they are unintuitively common. One way to intuit this is to consider the famous *birthday problem*.

**Problem Statement: The Birthday problem**

Given a group of $n$ people, find the probability that there is at least one pair of people with the same birthday.

Very unintuitively, the probably reaches 50% at just 23 people. At 367 people, the probability is 100% since there are only 366 possible birthdays. If we consider the analogy with respect to a hash table, we have a table of size 366, and with just 23 keys to insert, it is already more likely than not that a collision will occur. In general, with $n$ keys and a table of size $m$ where $n < m$, the probability that there exists a colliding pair is

$$p(n,m) = 1 - \frac{m!}{(m-n)!m^n}$$

which rapidly approaches 1 as $n \to m$. In practice, the best we can do is to minimise the probability of a collision by designing a good hash function. It is not realistic to try to avoid collisions 100% of the time, so the design of good hashtable data structures is therefore often heavily focused not only on avoiding collisions, but handling them in an efficient way when they do inevitably occur.

For the mathematically inclined, the rigorous analysis of hash collisions and complexity bounds on hashtables is analysed using tools from probabilistic combinatorics. Interested students should read *Probability and Computing*, Mitzenmacher & Upfal.

## Hashing Integers

The most common types of keys that we need to hash when implementing hashtables are integer types. Even when the types that we are dealing with might not be explicitly integers, there is often a simple and convenient way to interpret them as integers. For example, characters from a finite alphabet can be interpreted as integers corresponding to their position in the alphabet. A generalisation of this allows us to consider strings as integers in which we consider the characters as place values in some fixed radix system (covered in the next section.)

### The divisional method

The first and simplest method for producing a hash function for a set of integral keys onto a table of $m$ slots is to simply take the value of the key mod $m$. That is, for each key $k$, the hash function is

$$h(k) = k \mod m.$$

This hash function produces hash values that are usually well distributed provided that $m$ is selected well. In particular, one should take care to avoid using powers of two, since taking $k$ mod $2^p$ simply extracts the $p$ least significant bits of $k$. A good hash function should depend on the values of all of the bits in the key to increase the likelihood that the hashes are well distributed. Prime values of $m$, particularly those which are not close to a power of two are strong choices since some number theory will tell us that consecutive multiples of a key will continuously result in different hash values provided that the key is not a multiple of $m$ itself.

### The multiplicative method

The multiplicative hash works as follows. We select a constant $A$ where $A < 0 < 1$ and take the fractional part of $kA$, which is $kA - \lfloor kA \rfloor$. We then scale $m$ by the resulting value to produce a hash like so

$$h(k) = \lfloor m(kA - \lfloor kA \rfloor) \rfloor.$$

Unlike the divisional method, the value of $m$ does not heavily influence the quality of the hash, so taking $m$ as a power of two is fine and even preferable since the computation of the hash can then be sped up by taking advantage of bitwise operations.

The main decision to make is the value of $A$, whose optimal choice is heavily influenced by the characteristics of the keys being hashed. According to Knuth[1], a good choice is

$$A = \varphi^{-1} = \frac{\sqrt{5}-1}{2} \approx 0.61803...$$

[1] Donald E. Knuth. Sorting and Searching, volume 3 of *The Art of Computer Programming*. Addison-Wesley, 1973. Second edition, 1998

## Hashing Strings

The polynomial hashing technique is a common and effective method for hashing strings. Given a string $S[1..n]$, if we associate each character of $S$ with a numeric value (its position in the alphabet for example), then the polynomial hash is given by

$$h(S) = ((S[1]x^{n-1} + S[2]x^{n-2} + ... + S[n-1]x + S[n]) \mod p) \mod m,$$

where $p$ is a prime such that $p > m$. To reduce the chance of collisions, the value used for the base $x$ should be greater than the maximum attainable value of $S[i]$. If this is the case, then it is easy to see that the value of the polynomial hash for any string ignoring the modulo is unique, suggesting that this is a good hash function. Evaluating the polynomial hash for a given string naively term-by-term will lead to a time complexity of $O(n^2)$ or $O(n\log(n))$ if fast exponentiation is used, but this can be easily improved by using *Horner's Method*.

**Definition: Horner's Method**

Given the polynomial

$$p(x) = a_0 + a_1 x + a_2 x^2 + ... + a_n x^n$$

we can evaluate it in $O(n)$ time by computing the sequence of values

$$\begin{cases} b_n = a_n \\ b_{n-1} = a_{n-1} + b_n x \\ \vdots \\ b_0 = a_0 + b_1 x \end{cases}$$

where $b_0$ is the value of $p(x)$.

Horner's Method works because we can notice that a polynomial

$$p(x) = a_0 + a_1 x + a_2 x^2 + ... + a_n x^n$$

can be rewritten as

$$p(x) = a_0 + x(a_1 + x(a_2 + ... + x(a_{n-1} + a_n x))).$$

Horner's method then simply evaluates this expression from the innermost bracketed part outwards.

### Rolling the Polynomial Hash Function

One of the brilliant properties of the polynomial hash function that makes it so useful is that if we know the hash value of a particular substring of a given string, then we can compute the hash value of an adjacent substring (one differing in just one character) in just $O(1)$ time. Suppose that we first pre-compute the value of $x^{n-1}$ and we know the polynomial hash for some substring $S[i..j]$. Then the polynomial hash for the substring $S[i..j+1]$ is given by

$$h(S[i..j+1]) = ((x \times h(S[i..j]) + S[j+1]) \mod p) \mod m,$$

and the polynomial hash for the substring $S[i+1..j]$ can be computed as

$$h(S[i+1..j]) = ((h(S[i..j]) - S[i]x^{n-1}) \mod p) \mod m.$$

This allows us to "roll" the polynomial hash across a string and compute the hash values for all substrings of a fixed length in just linear time, rather than the quadratic time that would be required to do each substring separately.

## Universal Hashing (Not examinable in Semester Two, 2018)

All of our analysis above has assumed that our input keys are hashed uniformly at random to the table slots. This requires making among other things, the bold assumption that our input data is totally random. We should recall from our discussion of sorting that real world data is never random, so such assumptions are incorrect and foolish. When discussing Quicksort and Quickselect, a remarkably simple solution to combat the fact that our input data is not random was to choose our pivots randomly. Indeed, the simplest and most effective way to combat the fact that real-world data is not random is to introduce randomness into our algorithms instead! This ensures that no adversary can produce input that will cause our algorithms to run at worst-case performance. An ideal hash function would be *totally random*, that is, it would satisfy for all $x \in \mathcal{U}$, independent of all other elements of $\mathcal{U}$,

$$\Pr(h(x) = t) = \frac{1}{m}.$$

Unfortunately, generating a totally random hash function would require us to store a random hash value for every possible input key $x \in \mathcal{U}$, which would use just as much space as direct addressing! Instead, we try to approximate totally random hashing with hash functions that are somewhat random but easy to compute. One such approach is *universal hashing*.

In universal hashing, we select our hash function $h$ **randomly** from a *universal family* of hash functions. A family $\mathcal{H}$ is called universal if it satisfies

$$\Pr_{h \in \mathcal{H}} \{h(k) = h(k')\} \leq \frac{1}{m}, \qquad \text{for all } k \neq k' \in \mathcal{U}.$$

With universal hashing, the expected time per operation in chaining can be shown to still be $O(1+\alpha)$. Unfortunately, unlike totally random, universal hashing is not strong enough to guarantee that probing maintains $O(1)$ expected complexity. Here are three examples of universal families.

- The set $\mathcal{H}$ of all hash functions. This is clearly universal but it is completely useless since selecting from this family is equivalent to generating a totally random hash function which as we discussed is infeasible.
- $\mathcal{H} = \{h_{a,b}(k) = \big((ak+b) \mod p\big) \mod m\}$ for all $0 < a < p$, and all $0 \leq b < p$, for a fixed prime number such that $p \geq u$. This family has the disadvantage that table slots above $p$ mod $m$ may be less likely to be occupied. It is advantaged by the fact that it only needs to store three integers, $a$, $b$, and $p$ and hence uses very little space.

- $\mathscr{H} = \{h_{a,b}(k) = ((ak+b) \bmod u) >> (\log_2(u) - \log_2(m))\}$ for all odd $0 < a < u$, and all $0 \leq b < u/m$. This family works when $u$ and $m$, the universe size and the table size, are powers of two. This hash function then amounts to simply taking the highest $\log_2(m)$ bits from the product $(ak+b) \bmod u$, and is very fast to compute since when $m$ and $u$ are powers of two, no modular arithmetic is required, only bitwise operations and a single multiplication, which are much faster.

Even stronger families exist that provide stronger mathematical guarantees, but we won't discuss these for now[2].

## Cuckoo Hashing

Cuckoo hashing is a hashing scheme for hashtables that guarantees worst-case $O(1)$ lookup and deletion, while supporting $O(1)$ expected insertion assuming sufficiently good hash functions. The basic ideas are very simple. The tricky part is the analysis of whether insertion is fast.

**Key Ideas: Cuckoo Hashing**

1. Maintain two hashtables $T_1$ and $T_2$
2. Use two hash functions $f(k)$ and $g(k)$
3. If a collisions occurs, move the collided item to the other table

**To lookup a key $k$:**

1. Look at $T_1[f(k)]$, if found, return it
2. Look at $T_2[g(k)]$, if found return it
3. Otherwise, element not found

**Algorithm 34** Cuckoo hashing: Lookup

```
1: function LOOKUP(k)
2:     if T1[f(k)].key = x then return T1[f(k)]
3:     if T2[g(k)].key = x then return T2[g(k)]
4:     return null        // Not found
5: end function
```

**To delete an item with key $k$:**

1. Look at $T_1[f(k)]$, if found, delete it
2. Look at $T_2[g(k)]$, if found, delete it
3. Otherwise, element not found

[2] If interested, you should watch this lecture from MIT OpenCourseware, `https://youtu.be/Mf9Nn9PbGsE`.

**Algorithm 35** Cuckoo hashing: Deletion

```
1: function DELETE(item)
2:     if T1[f(item.key)] = item then T1[f(item.key)] = null
3:     else if T2[g(item.key)] = item then T2[g(item.key)] = null
4: end function
```

**To insert a key $k$:**

1. Attempt to insert the key $k$ into $T_1$ at position $f(k)$
2. If $k$ collides with an existing key in $T_1$, then move $k' = T_1[f(k)]$ into $T_2$ at position $g(k')$.
3. If moving $k'$ into $T_2$ caused a collision, take $k = T_2[g(k')]$ and attempt to insert it into $T_1$.
4. Continue until successful or until too many attempts have been made
5. If the process fails, rebuild the tables larger with new hash functions

**Algorithm 36** Cuckoo hashing: Insertion

```
1: function INSERT(item)
2:     if not LOOKUP(item.key) then       // Ignore if the key is already present
3:         for i = 1 to MaxLoop do
4:             swap(item, T1[f(item.key)])
5:             if item = null then return
6:             swap(item, T2[g(item.key)])
7:             if item = null then return
8:         end for
9:         rehash()       // Resize and start from scratch
10:        insert(item)       // Try again
11:    end if
12: end function
```

Lookup and deletion from a hashtable using cuckoo hashing clearly has a worst-case $O(1)$ complexity since it suffices to simply check two addresses. Analysis of insertion on the other hand is tricky. Selecting the appropriate threshold MaxLoop for insertion is important to ensure that rebuilds do not happen too frequently, but happen frequently enough such that insertions do not encounter too many probes. In theory, a good threshold to use is MaxLoop $= 6\log(n)$ with appropriate hash functions.

If the hash functions are assumed to be totally random and we maintain that the table sizes are $m \geq 2n$, then it can be shown that any given insertion will cause a failure with probability $O(1/n^2)$. Consequently, Cuckoo hashing will fail to insert $n$ keys with probability $O(1/n)$, which implies that $n$ keys can be inserted in expected $O(n)$ time. Unfortunately, Cuckoo hashing's downside is that it requires rather strong hash functions to achieve this complexity. Cuckoo hashing does not achieve $O(1)$ expected time with universal hashing, or even with some much stronger hash families[3].

[3]For the details and analysis, see Pagh & Rodler, Cuckoo Hashing, `http://www.it-c.dk/people/pagh/papers/cuckoo-jour.pdf` and/or this lecture from MIT OpenCourseware, `https://youtu.be/Mf9Nn9PbGsE`.

# Chapter 8

# Balanced Binary Search Trees

Storing and retrieving data is one of the most common scenarios in which we employ advanced data structures. We just covered hashtables which solve the dynamic dictionary problem in $O(1)$ expected time. You should already be familiar with binary search trees as a powerful alternative lookup data structure. Binary search trees are slower than hashtables in expectation, but they provide worst-case guarantees and can also support operations that hashtables are incapable of, like finding the elements closest to a given key. Ordinary binary search trees can, in the worst case degrade to $O(n)$ performance, so this chapter focuses on overcoming this weakness.

**Summary: Balanced Binary Search Trees**

In this chapter, we cover:

- Binary search trees
- AVL trees - Self-balancing binary search trees

**Recommended Resources: Balanced Binary Search Trees**

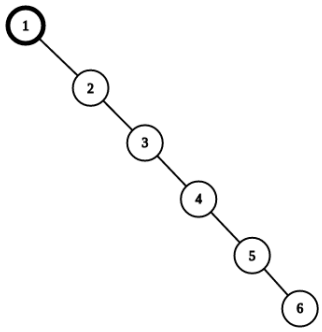
- CLRS, Introduction to Algorithms, Chapter 12
- Weiss, Data Structures and Algorithm Analysis, Chapter 4
- `https://visualgo.net/en/bst` - Visualisation of BSTs and AVL trees
- `https://people.ok.ubc.ca/ylucet/DS/AVLtree.html` - Visualisation
- `https://youtu.be/9Jry5-82I68` - MIT 6.006 lecture on binary search trees
- `https://youtu.be/FNeL18KsWPc` - MIT 6.006 lecture on AVL trees

## AVL Trees

Recall from your previous studies that a binary search tree is a rooted binary tree such that for each node, the keys in its left subtree compare less than its own and the keys in its right subtree compare greater than its own. Binary search trees are an efficient data structure for storing and retrieving elements of an ordered set in $O(\log(n))$ time per operation. Pathological cases can occur however when the tree becomes imbalanced, where performance degrades in the worst case to linear time. We will study one variety of improved binary search trees called an AVL[1] tree

[1] AVL trees are named after Adelson, Velskii, and Landis, the original inventors of the data structure.

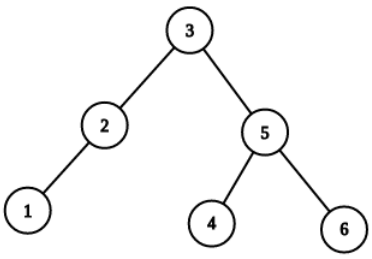
which self-adjusts to prevent imbalance and keeps all operations running in guaranteed worst case $O(\log(n))$ time.



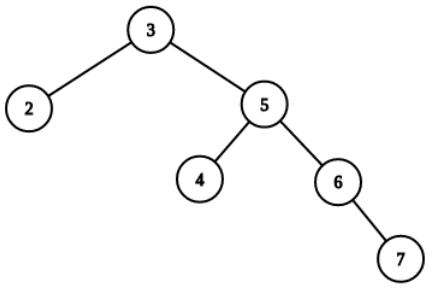

An example of a very imbalanced binary search tree resulting from inserting the keys $1,2,3,4,5,6$ in sorted order. Performance in such a tree is equivalent to a linked list with worst-case $O(n)$ lookup and insertion.

## Definitions

In general, a tree is considered balanced if it has a hight of $O(\log(n))$. There are many ways to achieve this with different kinds of trees. AVL trees use a very strict definition of balance which they maintain throughout insertions and deletions. In the context of an AVL tree, a tree is considered to be balanced if for any node in the tree, the heights of their left and right subtrees differ by at most one. This implies that its height is worst-case $O(\log(n))$, as required. Since lookup, insertion and deletion all take time proportional to the height of the tree, the tree being balanced implies that lookup, insertion and deletion can all be performed in worst-case $O(\log(n))$ time.




(a) Balanced




(b) Imbalanced

A balanced binary search tree (a) and an imbalanced binary search tree (b). (b) is imbalanced because the heights of the root node's left and right children are 1 and 3 respectively.

## Rebalancing

AVL trees maintain balance by performing *rotations* whenever an insertion or deletion operation violates the balance property. Rotations move some of the elements of the tree around in order to restore balance. We define the *balance factor* of a node to be the difference between the heights of its left and right subtrees, i.e.

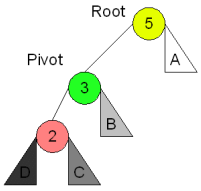
$$\text{balance\_factor(u)} = \text{height(u.left)} - \text{height(u.right)},$$

where height(**null**) = 0. A tree is therefore imbalanced if there is a node $u$ such that

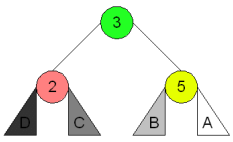
$$|\text{balance\_factor}(u)| \geq 2$$

There are four separate cases that can occur when a tree is imbalanced.

### Left-left imbalance



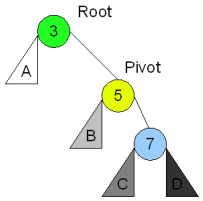

A left-left imbalance occurs when a node's balance factor is 2 (its left subtree is taller than its right subtree) and the left node's left subtree is at least as tall as the left node's right subtree (in other words, the balance factor of the left node is non-negative). To remedy a left-left imbalance, we perform a rightwards rotation, in which the left node becomes the new root, and the children are shifted accordingly. (Image source: Wikimedia Commons)



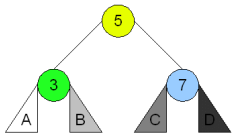

**Algorithm 37** AVL tree: Right rotation

```
1: function ROTATE_RIGHT(root)
2:     Set par = root.parent
3:     Set pivot = root.left
4:     Set temp = pivot.right
5:     pivot.set_right_child(root)
6:     root.set_left_child(temp)
7:     par.swap_child(root, pivot)
8: end function
```

### Right-right imbalance



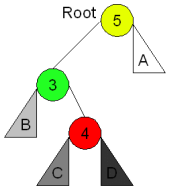

A right-right imbalance occurs when a node's balance factor is −2 (its right subtree is taller than its left subtree) and the right node's right subtree is at least as tall as the right node's left subtree (in other words, the balance factor of the right node is non-positive). To remedy a right-right imbalance, we perform a leftwards rotation, in which the right node becomes the new root, and the children are shifted accordingly. (Image source: Wikimedia Commons)



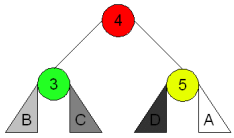

**Algorithm 38** AVL tree: Left rotation

```
1: function ROTATE_LEFT(root)
2:     Set par = root.parent
3:     Set pivot = root.right
4:     Set temp = pivot.left
5:     pivot.set_left_child(root)
6:     root.set_right_child(temp)
7:     par.swap_child(root, pivot)
8: end function
```

### Left-right imbalance



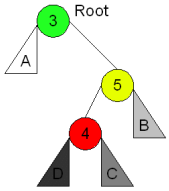

A left-right imbalance occurs when a node's balance factor is 2 (its left subtree is taller than its right subtree) and the left node's right subtree is taller than the left node's left subtree (in other words, the balance factor of the left node is negative). To remedy a left-right imbalance, we first perform a leftward rotation on the left node, which converts the imbalance into the left-left situation. We then perform a rightward rotation on the root to balance it. (Image source: Wikimedia Commons)



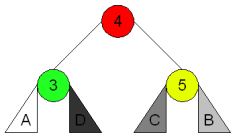

**Algorithm 39** AVL tree: Double-right rotation

```
1: function DOUBLE_ROTATE_RIGHT(root)
2:     rotate_left(root.left)
3:     rotate_right(root)
4: end function
```

### Right-left imbalance




A right-left imbalance occurs when a node's balance factor is −2 (its right subtree is taller than its left subtree) and the right node's left subtree is taller than the right node's right subtree (in other words, the balance factor of the right node is positive). To remedy a right-left imbalance, we first perform a rightward rotation on the right node, which converts the imbalance into the right-right situation. We then perform a leftward rotation on the root node to balance it. (Image source: Wikimedia Commons)




**Algorithm 40** AVL tree: Double-left rotation

```
1: function DOUBLE_ROTATE_LEFT(root)
2:     rotate_right(root.right)
3:     rotate_left(root)
4: end function
```

Note that in the above algorithms, it is crucial that the functions for manipulating the children also correctly update the node's parent pointers! Failing to do so is the most common bug that programmers encounter when attempting to implement self-balancing binary search trees. We should also make sure that we handle the null cases correctly when the children or the parent nodes are null. In implementations of self-balancing binary search trees, it is common to use special dummy nodes to represent null nodes rather than using the language's actual null pointer to avoid having to include special cases all throughout the code. We also have to store and maintain the heights of each node in the tree, since computing them online would be too slow.

Combining each of these together, the entire rebalancing procedure can be written as in Algorithm 41. After performing any modification to the tree, we should call rebalance on all ancestors of the modified nodes, starting with the deepest ones first. It is important to rebalance the deepest nodes first since fixing an imbalance at a low level of the tree may correct an imbalance higher up in the tree, eliminating the need for redundant rotations.

Since the tree is assumed to be balanced before we modify it, the heights of at most $O(\log(n))$ nodes are affected by any one modification operation and hence we require at most $O(\log(n))$ rebalances, each of which can be executed in constant time. Therefore the total time complexity of insertion and deletion for an AVL tree is worst-case $O(\log(n))$. Since the tree is kept balanced by the rebalances, lookup in the tree is also worst-case $O(\log(n))$.

**Algorithm 41** AVL tree: Rebalance

```
1: function REBALANCE(node)
2:     if balance_factor(node) = 2 then
3:         if balance_factor(node.left) < 0 then
4:             DOUBLE_ROTATE_RIGHT(node)
5:         else
6:             ROTATE_RIGHT(node)
7:         end if
8:     else if balance_factor(node) = -2 then
9:         if balance_factor(node.right) > 0 then
10:            DOUBLE_ROTATE_LEFT(node)
11:        else
12:            ROTATE_LEFT(node)
13:        end if
14:    end if
15: end function
```

# Chapter 9

# Prefix Tries and Suffix Trees

Today, huge amounts of the world's data is in the form of text data or data that can be interpreted as textual data. From classic literature, your favourite algorithms and data structures textbook to DNA sequences, text data is everywhere, and it needs to be stored, processed and analysed. We will introduce and study one special data structure for working with text strings, the suffix tree, as well as a related data structure, the prefix trie / retrieval tree data structure which allows for fast storage and lookup of strings.

**Summary: Prefix Tries and Suffix Trees**

In this chapter, we cover:

- Retrieval Trees / Prefix Tries
- Suffix trees
- Applications of suffix trees

**Recommended Resources: Prefix Tries and Suffix Trees**

- Weiss, Data Structures and Algorithm Analysis, Section 12.4.2
- `https://www.cs.usfca.edu/~galles/visualization/Trie.html` - Tries
- `https://visualgo.net/suffixtree` - Visualisation of suffix trees
- `https://youtu.be/NinWEPPrkDQ` - MIT 6.851 lecture on string data structures
- `http://www.allisons.org/ll/AlgDS/Tree/Suffix/`

## String Terminology

Recall that a *string* $S[1..n]$ is a sequence of characters, i.e. some textual data.

1. A *substring* of $S$ is a string $S[i..j]$ where $1 \leq i \leq j \leq n$.
2. A *prefix* of $S$ is a substring $S[1..j]$ where $1 \leq j \leq n$.
3. A *suffix* of $S$ is a substring $S[i..n]$ where $1 \leq i \leq n$.

A useful observation to make is that a substring of $S$ is always a prefix of some suffix of $S$.

## The Prefix Trie / Retrieval Tree Data Structure

A retrieval tree or prefix trie is a data structure that stores a set of strings arranged in a tree such that words with a shared prefix are contained within the same subtree.

**Key Ideas: Prefix Trie**

- The prefix trie is a rooted tree (not necessarily binary)
- Each edge of the tree is labelled with a character. Alternatively, each node (except the root) can be labelled, which is equivalent to labelling its parent edge.
- A path from the root to a node in the trie corresponds to a prefix of a word in the trie
- A path from the root to an internal node of the trie corresponds to a common prefix of multiple strings

Prefix tries can be implemented in a variety of ways. The most important decision is how to index the children of a particular node. There are a several strategies, and we will consider three of them. We will denote the length of a query string by $n$, the total length of all words in the trie by $T$, and the alphabet by $\Sigma$.

- Use an array to store a child pointer for each character in the alphabet:

  This method allows us to perform lookup and insert in $O(n)$ time since we can follow each child pointer in constant time. However, the space requirement is quite high, since we are storing a lot of pointers to null children. Specifically, we will use $O(|\Sigma|T)$ space in the worse case, since every node has a pointer for every character in the alphabet.

- Use a balanced binary search tree for storing child pointers:

  This method uses the minimal amount of space, as we only need to store pointers to children that actually exist. For large alphabets, this is advantageous. However, we lose in lookup time since it now requires up to $O(n\log(|\Sigma|))$ time per lookup since at each node we must search a BST to find the child pointer. The total space requirement however is minimal, at just $O(T)$.

- Use a hashtable for storing child pointers:

  This method allows us to only store pointers to the children that exist, hence we will only use the minimal $O(T)$ space. It also allows lookup in $O(n)$ expected time, since at each node we perform a hashtable lookup in expected constant time. This method seems to be superior to the first two since it has optimal speed and optimal space usage. However, this implementation is less versatile, and prohibits us from doing some more advanced tricks with the trie. For example, you might want to implement the ability to lookup the alphabetically closest word to a given word. This is possible with the first two approaches, but not (efficiently) with a hashtable since there is no way in a hashtable to quickly lookup the alphabetically nearest key. It also does not provide worst-case guarantees which might be important to us.

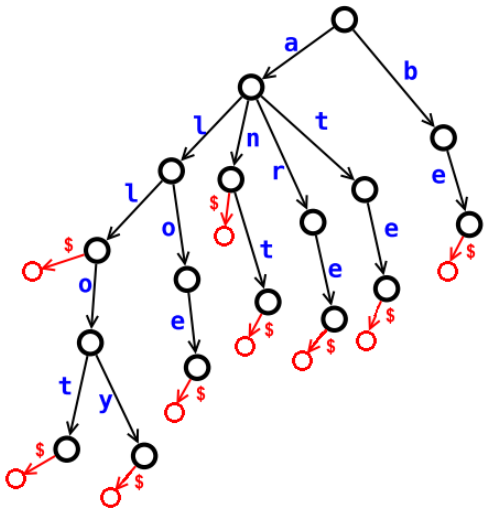



Figure 9.1: An example of a prefix trie containing the strings `be`, `ant`, `alloy`, `ate`, `are`, `aloe`, `an`, `allot`, `all`, with terminating $ characters added to indicate the ends of words.

It is common to terminate each word with a special character to allow us to distinguish between full words and prefixes. This special character is usually denoted by $. This ensures that a node is a leaf if and only if it is the end of a word. In actual code, you should use the null character (`'\0'` in ASCII) rather than an actual $ since $ may be a character in one of the strings.

## Applications of tries

### Prefix matching / exact string lookup

Prefix tries are designed to solve the prefix matching problem, i.e. determining whether a list of strings contains a word that begins with a particular prefix. If we terminate all words a $\$ \notin \Sigma$, then we also gain the ability to do exact searches by appending $ to our query strings, since $ will not be contained in any proper prefix of a word. This makes tries a potential substitute for a hashtable for storing a dictionary of strings. Implementations of insertion and lookup for prefix tries are shown in Algorithms 42 and 43 respectively. If we use the array-based implementation, building a prefix trie takes $O(|\Sigma|T)$ time, and lookup takes $O(n)$ time, which are optimal if $|\Sigma|$ is constant.

### Sorting a list of strings

We can use a prefix trie to quickly sort a list of strings coming from a fixed size alphabet. Simply insert all of the strings into a prefix trie, and then traverse the trie in lexicographical order. Using the array-based implementation, the complexity of this algorithm is $O(|\Sigma|T)$. If we used the balanced-binary-search-tree-based implementation instead, we could reduce the complexity

**Algorithm 42** Prefix trie: Insertion

```
1:  function INSERT(S[1..n])
2:      Set node = root
3:      for each character c in S[1..n] do
4:          if node has an edge for character c then
5:              node = node.get_child(c)
6:          else
7:              node = node.create_child(c)
8:          end if
9:      end for
10: end function
```

**Algorithm 43** Prefix trie: Lookup

```
1:  // Returns True if the trie contains a word that has S as a prefix
2:  function LOOKUP(S[1..n])
3:      Set node = root
4:      for each character c in S[1..n] do
5:          if node has an edge for character c then
6:              node = node.get_child(c)
7:          else
8:              return False
9:          end if
10:     end for
11:     return True
12: end function
```

to $O(T\log(|\Sigma|))$. Assuming that all of the input strings are roughly the same length, the complexity of sorting the strings using a typical fast sorting algorithm would instead be

$$O(n\log(n)) \times O\left(\frac{T}{n}\right) = O(T\log(n)),$$

where $n$ is the number of words in the list being sorted. We can therefore see that if the alphabet size is constant or sufficiently small, the prefix trie method will be faster. Lastly, note that this is actually a form of radix sort, specifically a most significant digit (MSD) radix sort, since strings are divided up based on their characters, first to last as we go down the tree. An implementation of sorting using a trie is given in Algorithm 44.

## Compact Tries (Not examinable in Semester Two, 2018)

One major drawback to tries that we have observed is that they can potentially waste a lot of memory, particularly if they contain long non-branching paths (paths where each node only has one child). In cases like these, we can make prefix tries more efficient by combining the edges along a non-branching path into a single edge. The *Radix Trie* and the *PATRICIA Trie* are particular kinds of compact prefix tries. Figure 9.2 shows an example of a compact trie.

**Algorithm 44** Prefix trie: String sorting

```
1:  function SORT_STRINGS(strings[1..n])
2:      for each string s in strings[1..n] do
3:          INSERT(s + '$')
4:      end for
5:      TRAVERSE(root, "")
6:  end function
7:
8:  function TRAVERSE(node, cur_string)
9:      if cur_strings ends with '$' then        // We are at the end of a string
10:         print (cur_string)        // Can omit printing the '$' character
11:     else
12:         for each child character c of node in alphabetical order do
13:             cur_string.append(c)
14:             TRAVERSE(node.get_child(c), cur_string)
15:             cur_string.pop_back()        // Remove the last character of cur_string
16:         end for
17:     end if
18: end function
```

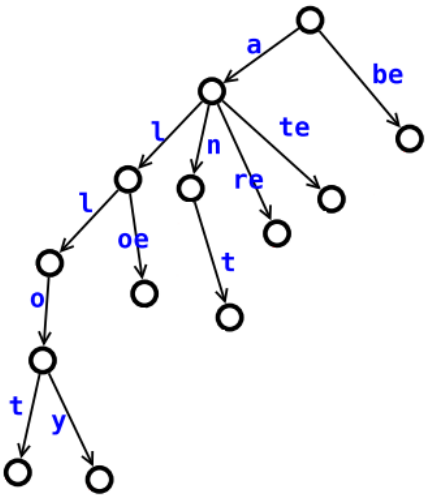



Figure 9.2: A compact trie containing `be`, `ant`, `alloy`, `ate`, `are`, `aloe`, `an`, `allot`, `all`. No terminating character $ has been added in this example.

## Suffix Trees

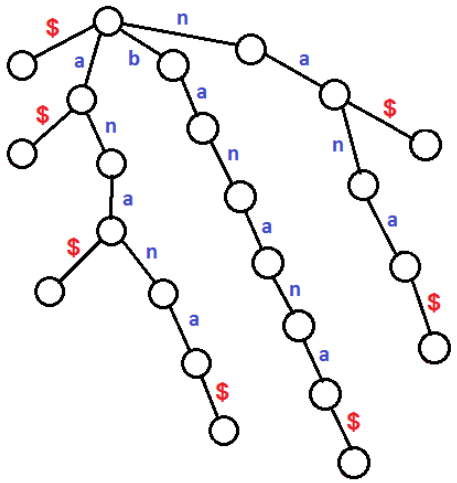
A suffix tree is a compact trie containing all of the suffixes of a string. We motivate suffix trees as a solution to the *pattern matching* problem.

**Problem Statement: Pattern matching**

Given a text string $T[1..n]$ and a pattern $P[1..m]$, find all occurrences of $P$ as a substring of $T$.

Many well known algorithms exist that will solve the pattern matching problem in $O(n+m)$ per query, but what if we wish to keep the same text string $T$ and search for lots of small patterns? Doing the $O(n)$ work per query might turn out to be extremely wasteful if the text string has length $n = 1,000,000$ and the patterns only have length $m = 20$.

We can start with a *suffix trie* by inserting all of the suffixes into a prefix trie. In many applications, we need to be able to distinguish suffixes from substrings so we add the terminating character \$.




A suffix trie for the string "banana\$".

A suffix trie of the string $T$ can be used to solve the pattern matching problem by checking whether $P$ is a prefix in the trie. This will take $O(m)$ time per query, which is optimal. Since a string of length $n$ has $n$ suffixes, and each has length $O(n)$, a suffix trie will take $O(n^2)$ space, which is extremely inefficient. This is why the suffix tree is stored as a compact trie, which will take just $O(n)$ space. A suffix tree of the string `banana$` is shown in Figure 9.3.

It is important to note that if we store all of the edge labels explicitly then the memory used by the suffix tree will still be $O(n^2)$. In order to mitigate this and bring the memory required down to $O(n)$, we instead simply refer to each substring by its position in the original string. For example, the substring "na" in "banana\$" would simply be represented as $[3,4]$, meaning that it is the substring spanning the positions 3 to 4 in the string "banana\$".

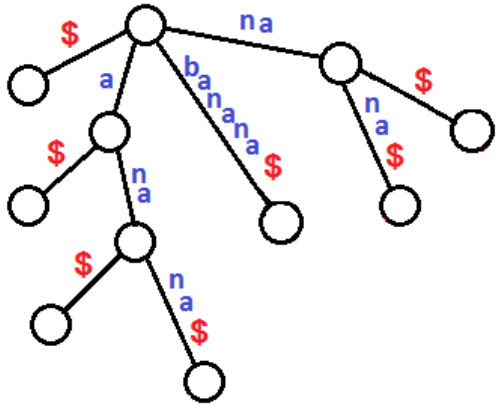



Figure 9.3: A suffix tree for the string “banana$”.

## Building a suffix tree

### The naive approach

The simplest way to build a suffix tree is to build the suffix trie in $O(n^2)$ and then compress it into a suffix tree. This is simple to implement but is unfortunately useless in practice due to the poor time complexity.

### Converting from Suffix Array (Not examinable in Semester Two, 2018)

In the next lecture, we will learn about another data structure, the suffix array. Suffix arrays encode the relative lexicographical order of all of the suffixes off a string. Interestingly, suffix arrays and suffix trees actually encode precisely the same information. That is, given the suffix array of a particular string and the string itself, you can determine the suffix tree, and vice versa. The first idea is to notice that compressed branches in the suffix tree correspond to *longest common prefixes* between suffixes, which can be computed from the suffix array by cleverly comparing adjacent suffixes. These suffixes can then be inserted as a branch into the suffix tree recursively. Using a data structure called a Cartesian tree, this whole process can be done in just $O(n)$ time. Since suffix arrays can be computed in $O(n)$ time and the longest common prefixes can be computed in $O(n)$ time, this yields a rather obtuse but nonetheless $O(n)$ algorithm for building a suffix tree.

### Ukkonen’s algorithm (Not examinable in Semester Two, 2018)

A very elegant algorithm for constructing suffix trees was given by Ukkonen[1], who produced an algorithm that was not only $O(n)$ time but also **online**, meaning that you can continue to add characters to the string while updating the suffix tree without having to start over from scratch.

[1]If interested, see E Ukkonen, On-line construction of suffix trees, *Algorithmica* 1995, and this Stackoverflow post `http://stackoverflow.com/questions/9452701` which describes the algorithm in a very accessible way.

In its essence, Ukkonen's algorithm works by extending the length of each leaf edge of the suffix tree by one for each new character inserted, and appropriately splitting existing edges into two whenever a common prefix diverges.

## Applications of suffix trees

### Pattern matching

Since we could use the suffix trie to perform pattern matching in $O(m)$ time, we can also use the suffix tree for pattern matching in exactly the same way. The implementation is a little more involved since traversing the suffix tree along the edges requires more work (to check that each character along the edge is a match), but the idea and complexity are the same.

### The longest repeated substring problem

**Problem Statement: Longest repeated substring**

Given a string $S[1..n]$, find the longest substring of $S$ that occurs at least two times.

To solve this problem, we recall that within a prefix trie and equivalently a suffix tree, internal nodes correspond precisely to common prefixes, and hence in the case of suffix trees, substrings that occur multiple times. Finding the longest repeated substring is therefore simply a matter of traversing the suffix tree and looking for the deepest internal node (non-leaf node). An example is depicted in Figure 9.4.

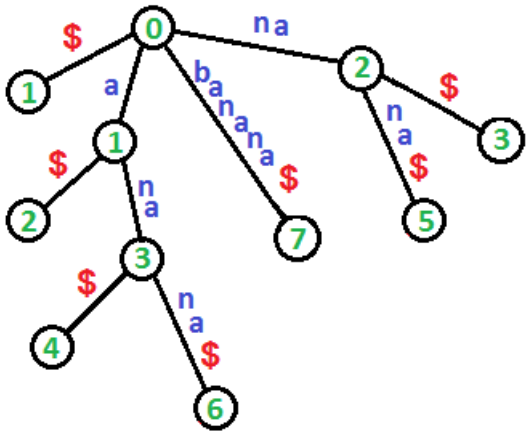



Figure 9.4: A suffix tree for the string "banana$" where each node is labelled with its depth (distance from the root node as measured by the number of characters on each edge). The deepest internal node has depth 3, which corresponds to the substring "ana."

# Chapter 10

# Suffix Arrays

We just saw the suffix tree data structure, a compact structure for processing and answering questions about strings. In addition to the suffix tree, there are many other data structures that utilise the suffixes of a string to perform efficient string related queries. We will study one more such structure as a more space efficient alternative to the suffix tree, the suffix array.

**Summary: Suffix Arrays**

In this chapter, we cover:

- Suffix arrays
- How to build a suffix array
- Applications of suffix arrays

**Recommended Resources: Suffix Arrays**

- Weiss, Data Structures and Algorithm Analysis, Section 12.4.1
- `https://youtu.be/NinWEPPrkDQ` - MIT 6.851 lecture on string data structures
- `https://visualgo.net/suffixarray` - Visualisation of suffix arrays
- `http://www.allisons.org/ll/AlgDS/Strings/Suffix/`

## Suffix Arrays

Suffix arrays are a compact data structure that index all of the suffixes of a particular string in sorted order. While this may not sound immediately useful at first sight, the suffix array has a mountain of applications in string processing which carry over to applications in fields ranging from the study of natural languages to bioinformatics.

Consider as a first example, the string `banana`. Recall that when working with suffixes, we often mark the end of the string with a special character, denoted by $. The suffixes of `banana$` are then given by

```
banana$
anana$
nana$
ana$
na$
a$
$
```

In general, we can see that a string of length $n$ has $n+1$ suffixes (including the empty suffix containing only \$.) The suffix array of a string is a sorted array of its suffixes, so the suffix array of banana looks like

```
$
a$
ana$
anana$
banana$
na$
nana$
```

Note that the special character (\$) is considered to be lexicographically less than all other suffixes, so it appears at the beginning of the suffix array. This is useful since it conceptually signifies the *empty string* (the suffix of length zero of the original string.)

Since actually writing down all of the suffixes of a string would take $O(n^2)$ space, suffix arrays are represented in a more compact form, where each element simply refers to an index $1 \leq i \leq n$ into S at which the corresponding suffix begins. For example, the suffix array for `banana` would be stored as:

$$\text{SA("banana\$")} = [7,6,4,2,1,5,3]$$

where the $i^{\text{th}}$ index corresponds to the position in `banana` at which the $i^{\text{th}}$ sorted suffix starts as shown in the table bellow.

| **Index** | **Suffix** |
|---|---|
| 7 | `$` |
| 6 | `a$` |
| 4 | `ana$` |
| 2 | `anana$` |
| 1 | `banana$` |
| 5 | `na$` |
| 3 | `nana$` |

In practice, the first entry (7 in this case) is sometimes omitted since it is guaranteed that the empty suffix is always the first one.

# Building a Suffix Array

## The naive approach

The simplest and most obvious way to build a suffix array is to simply build a list containing the indices $1..n$ and to sort them by comparing suffixes. Although short and simple, this implementation is useless in practice since its time complexity is $O(n^2 \log(n))$, owing to the fact that sorting performs $O(n \log(n))$ comparisons and each pair of suffixes takes $O(n)$ time to compare, which means that this algorithm can not be used on large strings. An implementation is show in Algorithm 45.

**Algorithm 45** Naive suffix array construction

```
1:  function SUFFIX_ARRAY(S[1..n])
2:      Set SA[1..n] = [1..n]
3:      sort(SA[1..n], suffix_compare(S, ...))      // Use suffix_compare as the comparison operator
4:      return SA
5:  end function
6:
7:  // Compare the suffixes at position i and j
8:  function SUFFIX_COMPARE(S[1..n], i, j)
9:      return (S[i..n] < S[j..n])
10: end function
```

## The prefix doubling algorithm

The naive algorithm for constructing suffix arrays is simply too slow to work on large strings. A much faster approach which is still conceptually simple is the *prefix doubling* algorithm.

**Key Ideas: Prefix Doubling Algorithm**

To construct the suffix array of the string $S[1..n]$

1. Sort the suffixes by their first character
2. Sort the suffixes by their first two characters
3. Sort the suffixes by their first four characters
4. ...
5. Sort the suffixes by their first $k$ characters ($k$ = a power of two)
6. Sort the suffixes by their first $2k$ characters

**Note:** If a suffix beginning at a particular position has length less than $k$ at a particular iteration, it is considered to have empty characters coming after it, remembering that the empty character compares less than all others, e.g. “cat” < “cathode.”

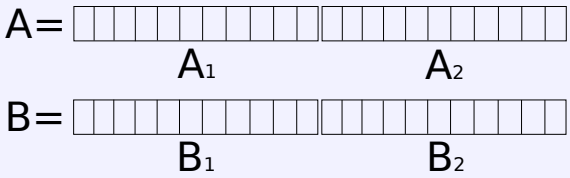
What we are really doing here is sorting consecutively larger prefixes of the suffixes, hence the name prefix doubling. If we perform prefix doubling naively by simply comparing substrings at each iteration, this will be no faster than the naive algorithm (in fact it will be even slower!) We therefore need a trick to perform the comparisons faster.

#### Fast suffix comparison

Prefix doubling iteratively sorts longer and longer substrings each round. The key idea is that by knowing the sorted order of the shorter substrings, we can compare the longer substrings fast!

**Key Ideas: Fast suffix comparison**

Suppose we wish to compare two strings $A$ and $B$, each of which has the same even length. We can imagine these two strings as being composed of two halves. Call these halves $A_1, A_2$ and $B_1, B_2$.




When we compare $A$ and $B$ naively, we are comparing them from character 1 through to character $l$ in order until we hit a pair of letters that differ. What if we already know that $A_1 < B_1$? This means that the first pair of characters that differ between $A$ and $B$ occurs in the first half in favour of $A$, and therefore $A < B$. We don't even have to look at the second halves. If instead we knew that $A_1 > B_1$, then we would similarly know that $A > B$.

If instead $A_1 = B_1$, then there is no point comparing the characters in the first halves of $A$ and $B$ since we already know that they must be the same. We can then apply the same logic to $A_2$ and $B_2$ and deduce that if $A_2 < B_2$ then $A < B$, or if $A_2 > B_2$ that $A > B$, or finally if $A_2 = B_2$ that $A = B$. What this tells us is that knowing the order of the halves of the strings we are comparing allows us to skip comparing all of the characters. In fact, all we had to do was compare the halves, so we only had to do at most 2 comparisons, regardless of the lengths of $A$ and $B$! This means we can perform comparisons in $O(1)$ if we already know the sorted order of the halves.

For example, say we wish to compare the long strings "supercalafragalisticexpialadoshs" and "supercalafragalisticsuffixarrays". Comparing them naively, we would take until character 21 to find the answer. However, if we were to look at the strings as made up of two halves:

```
``supercalafragali''+``sticexpialadoshs''
``supercalafragali''+``sticsuffixarrays''
```

and I were to tell you that the first halves are the same, and that the second half of the first string "sticexpialadoshs" is less than the second half of the second string "sticsuffixarrays", you could

immediately tell me that the first string is less than the second.

This explains why prefix doubling sorts the first 1 character, then 2 characters, then 4 and so on. What is important to realise here is that if I am looking at the first $2k$ characters of the suffix at position $p$, then what I really have are two halves: the first $k$ characters of the suffix at position $p$ and the first $k$ characters of the suffix at position $p+k$. At each iteration, knowing the order of the previous halves allows all of the comparisons of the current suffixes to be performed in $O(1)$ time.

#### Maintaining the sorted order

The last issue that we must discuss before presenting the entire prefix doubling algorithm is keeping track of the sorted order of the suffixes. We know that the key piece of information we need is to be able to compare two halves quickly. If we have all of the suffixes partially sorted, then we can compare two of them by searching the array and seeing which one comes first, but this would take $O(n)$ time and negate all of the hard work that prefix doubling is doing for us. Instead, we need to maintain a second array, the *rank* array. The rank array remembers for each suffix, its current position in the suffix array. Two suffixes that are equal up to the current length must be assigned the same rank so that we know that they are equal. For example, say we are computing the suffix array of "banana" and we have already sorted on the first two characters of each suffix and are now about to compare on the first four characters of each suffix. The partially sorted suffixes and their ranks are

| **Index** | **Suffix** | **Rank** |
|---|---|---|
| 7 | **$** | 1 |
| 6 | **a$** | 2 |
| 2 | **an**ana$ | 3 |
| 4 | **an**a$ | 3 |
| 1 | **ba**nana$ | 4 |
| 3 | **na**na$ | 5 |
| 5 | **na**$ | 5 |

and hence the partially sorted suffix array and the rank array would look like

| Index | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|---|
| Suffix Array | 7 | 6 | 2 | 4 | 1 | 3 | 5 |
| Rank | 4 | 3 | 5 | 3 | 5 | 2 | 1 |

If we know the ranks of two suffixes, we can compare them by simply comparing their ranks, since a lower rank means it comes earlier in the suffix array. We now have all of the ingredients to implement prefix doubling.

### Implementation of Prefix Doubling

An implementation of prefix doubling is given in Algorithm 46. The value `ord(c)` simply refers to the order or rank of the character `c` in the alphabet. e.g. `ord('a') = 1`, `ord('b') = 2`, etc. The SUFFIX_COMPARE function compares two prefixes of length $k$ in $O(1)$ by looking at the ranks of the two halves of the prefix, i.e. it compares by the pairs $(\text{rank}[i], \text{rank}[i+k])$. After sorting, we compute the new ranks by going through the suffixes in the current order, and adding 1 to the rank if the current suffix is greater than the previous one. This ensures that we correctly assign equal ranks to suffixes that are currently equal. Sorting at each iteration of the algorithm takes $O(n\log(n))$ time since the comparisons are now performed in $O(1)$, and we have to perform $\log(n)$ iterations to fully sort the suffixes, so the total time complexity of the prefix doubling algorithm is $O(n\log^2(n))$.

**Algorithm 46** Prefix-doubling suffix array construction

```
1:  function SUFFIX_ARRAY(S[1..n])
2:      Set SA[1..n] = [1..n]
3:      Set rank[1..n] = [ord(S[1..n])]
4:      for k = 1 to n, stepping k *= 2 do
5:          sort(SA[1..n], suffix_compare(rank, k, ...))
6:          // Update the rank array to account for the new sorted order
7:          Set temp[1..n] = 0
8:          for i = 1 to n-1 do
9:              temp[SA[i+1]] = temp[SA[i]] + suffix_compare(rank[1..n], k, SA[i], SA[i+1])
10:         end for
11:         swap(temp, rank)
12:     end for
13:     return SA
14: end function
15:
16: // Compare the suffixes of length 2k beginning at positions i and j
17: function SUFFIX_COMPARE(rank[1..n], k, i, j)
18:     if rank[i] ≠ rank[j] then        // Compare by first halves
19:         return rank[i] < rank[j]
20:     else if i+k ≤ n and j+k ≤ n then        // Compare by second halves
21:         return rank[i+k] < rank[j+k]
22:     else        // Second half is empty
23:         return j < i
24:     end if
25: end function
```

## Speeding up prefix doubling (Not examinable in Semester Two, 2018)

The prefix doubling algorithm is already significantly faster than the naive suffix array construction method, but there is still lots of room for improvement. Since the ranks are bounded above by $n$, we can speed up prefix doubling by replacing the $O(n\log(n))$ sort with an $O(n)$ radix sort instead. To take advantage of radix sort, we interpret prefix doubling as sorting suffixes using

the pairs $(\text{rank}[i], \text{rank}[i+k])$ as the keys, since these correspond to the two halves of the $i^{\text{th}}$ suffix of length $2k$. We can therefore sort the array by first sorting on $\text{rank}[i+k]$ and then stably sorting on $\text{rank}[i]$. Using a counting sort for each of these, we perform $O(n)$ work to sort the array. Using this method, the complexity of the prefix doubling algorithm drops to $O(n \log(n))$ since we still perform $O(\log(n))$ rounds, but each round now takes just $O(n)$.

### Linear time suffix arrays (Not examinable in Semester Two, 2018)

Prefix doubling with radix sort achieves reasonably good performance on very large strings in practice, but we can still do even better! Several algorithms exist for constructing suffix arrays in just $O(n)$ time for a fixed size alphabet. Probably the most well known of these algorithms is the DC3 algorithm[1], which works by sorting a set of "sample suffixes" which are the suffixes at positions in the string that are not divisible by three. DC3 operates by radix sorting the first three characters of each suffix (stably in reverse order), then recursively sorting sets of suffixes that are still equal. Using the sample suffixes, one can then quickly sort the remaining $1/3$ of the suffixes and merge them with the sample suffixes since every non-sample suffix is just one character prepended to a sample suffix. The running time is then given by

$$T(n) = \begin{cases} T\left(\frac{2}{3}n\right) + O(n) & \text{if } n > 1, \\ \Theta(1) & \text{if } n = 1. \end{cases}$$

which can be solved to reveal a time complexity of $O(n)$.

## Applications of Suffix Arrays

As fun as suffix arrays are to think about, they also admit a wide range of useful applications to string processing problems. Let's look at the most important one, pattern matching.

### Pattern matching with suffix arrays

Using the suffix array of the text string $T[1..n]$, we can perform pattern searches fast, saving time if a large number of searches on the same string are desired. The idea is very simple: since the suffix array gives the suffixes in sorted order, all occurrences of the pattern that we are searching for will exist in some contiguous range. Since they are sorted, we can find this range with a pair of binary searches, one to locate the first occurrence and one to locate the final occurrence. The idea is illustrated in Algorithm 47. All of the occurrences of the pattern are found at the positions given by `SA[begin..end]`. If this range is empty, then no matches were found. Since each string comparison takes $O(m)$ time and the binary searches must perform $O(\log(n))$ iterations, the total time complexity of pattern matching using a suffix array is $O(m \log(n))$ which is a significant improvement over $O(n+m)$ when $n \gg m$. It is possible to speed this up to just $O(m)$ using the *longest common prefix array*, a companion to the suffix array which we will not cover for now.

[1] See *Linear Work Suffix Array Construction* , Juha Kärkkäinen, Peter Sanders, Stefan Burkhardt

**Algorithm 47** Suffix array: Pattern matching

```
1:  function FIND_PATTERN(SA[1..n], T[1..n], P[1..m])
2:      // Binary search to find the first occurrence of P
3:      // Invariant: T[SA[lo]..n] < P and T[SA[hi]..n] ≥ P
4:      Set lo = 0, hi = n
5:      while lo < hi - 1 do
6:          Set mid = ⌊(lo + hi)/2⌋
7:          if T[SA[mid]..n] < P[1..m] then
8:              lo = mid
9:          else
10:             hi = mid
11:         end if
12:     end while
13:     Set begin = hi
14:     // Binary search to find the final occurrence of P
15:     // Invariant: T[SA[lo]..n] ≤ P and T[SA[hi]..n] < P
16:     lo = 1, hi = n + 1
17:     while lo < hi - 1 do
18:         Set mid = ⌊(lo + hi)/2⌋
19:         if T[SA[mid]..n] ≤ P[1..m] then
20:             lo = mid
21:         else
22:             hi = mid
23:         end if
24:     end while
25:     Set end = lo
26:     return begin, end
27: end function
```

# Chapter 11

# The Burrows-Wheeler Transform

Two of the most common problems that arise in string processing are text compression and pattern matching. We've already seen two data structures for performing pattern matching, each with different advantages and disadvantages. The Burrows-Wheeler transform is a string transformation with powerful applications to text compression and pattern matching on very large strings.

**Summary: The Burrows-Wheeler transform**

In this chapter, we cover:

- The Burrows-Wheeler transform of a string
- The inverse Burrows-Wheeler transform
- The application of BWT to pattern matching

**Recommended Resources: The Burrows-Wheeler transform**

- Michael Burrows and David J Wheeler. A block-sorting lossless data compression algorithm. 1994

## The Burrows-Wheeler Transform

The Burrows-Wheeler transform (BWT) of a string is a permutation of the characters in that string that often improves the compressibility of the resulting string and facilitates fast pattern matching.

**Definition: The Burrows-Wheeler transform**

The Burrows-Wheeler transform of a string $S[1..n]$ is a string formed by taking the final character of each cyclic permutation of $S$+'$' arranged in sorted order.

Let's make this clearer with an example. Consider our favourite string "banana$", remembering that we use the special $ symbol to denote the end of the string, and that it is considered lexicographically less than any other character in the alphabet. The *cyclic permutations* of a string are the permutations of that string that can be obtained by rotating the elements in a cyclic order. For example, the cyclic permutations of "banana$" are

```
banana$
anana$b
nana$ba
ana$ban
na$bana
a$banan
$banana
```

For a string of length $n$, there are exactly $n$ cyclic permutations, given by

$$S[i..n]+S[1..i-1], \qquad \text{for } i = 1 \text{ to } n,$$

where $S[...]+S[...]$ denotes a string concatenation. To obtain the BWT of a string, we sort these cyclic permutation in lexicographical order. For "banana$", this gives us

```
$banana
a$banan
ana$ban
anana$b
banana$
na$bana
nana$ba
```

The BWT of "banana$" is the string formed by taking the final character of each of these sorted cyclic permutations, so we have

$$\text{BWT}(\texttt{"banana\$"}) = \texttt{"annb\$aa"}$$

We will refer to the $n \times n$ matrix of characters of the sorted cyclic shifts as the BWT matrix $M$.

## Useful properties of the BWT

**Property 1: The last column of the BWT matrix precedes the first column**

Since $M$ contains the sorted cyclic permutations of $S[1..n]$, the contents of the last column of $M$ are precisely the characters that cyclically precede the characters in the first column. **This might seem unspectacular, but this is the most important property of the BWT which underpins many of the following observations and subsequent algorithms that we will derive. Make sure this sinks in before moving forward.**

**Property 2: BWT groups runs of similar characters**

We can see in the BWT of "banana$", that the transformed text often consists of groups of repeated characters. This makes BWT very useful for **text compression** methods that take advantage of repeated characters.

**Property 3: The BWT matrix contains permutations of all the k-mers of $S[1..n]$**

The BWT matrix is the matrix of all sorted cyclic permutations of $S[1..n]$. For example, the BWT matrix for "banana$" is

$$M = \begin{bmatrix} \$ & b & a & n & a & n & a \\ a & \$ & b & a & n & a & n \\ a & n & a & \$ & b & a & n \\ a & n & a & n & a & \$ & b \\ b & a & n & a & n & a & \$ \\ n & a & \$ & b & a & n & a \\ n & a & n & a & \$ & b & a \end{bmatrix}$$

Notice that the BWT of $S[1..n]$ is the string formed by the final column of $M$. Also, we can see from that above matrix that

1. Every column of $M$ is a permutation of $S[1..n]$
2. Every pair of adjacent columns of $M$ contains a permutation of all of the length 2 substrings of $S[1..n]$ (also called 2-mers of $S$)
3. Every sequence of $k$ consecutive columns of $M$ contains a permutation of all of the length $k$ substrings of $S[1..n]$ (called the $k$-mers of $S$)

This observation may not seem obviously useful yet, but it underpins the **pattern matching** algorithm that utilises BWT later.

**Property 4: The BWT is invertible**

Given the BWT of a string BWT($S[1..n]$), it is possible to transform back to the original text $S[1..n]$ without any extra information. In particular, this means that compression methods can take advantage of BWT without lots of space overhead, i.e. you pay only a single byte (the addition of the $ character) of extra space to improve the compressibility of the string.

## Computation of the BWT

Clearly we can compute the BTW of a string in $O(n^2 \log(n))$ time by simply storing all of the cyclic permutations in a list, sorting them using a fast sorting algorithm and then taking the last character of each. This is far too slow in practice, so better methods for computing the BTW are used. The key observation to make is that because the terminating character $ is lexicographically less than all other characters, the order of the cyclic permutations is precisely the same order as the sorted suffixes of the string.

$banana
a$banan
ana$ban
anana$b
banana$
na$bana
nana$ba

Notice that the characters in black are exactly the sorted suffixes. This means that we can use the suffix array to compute the BWT efficiently.

**Algorithm 48** Burrows-Wheeler transform

```
1: function BWT(S[1..n])
2:     Set SA[1..n] = SUFFIX_ARRAY(S)
3:     Set result[1..n] = {}
4:     for i = 1 to n do
5:         result[i] = S[SA[i]-1] or '$' if SA[i] = 1
6:     end for
7:     return result
8: end function
```

Since suffix arrays can be computed in linear time, this implies that the Burrows-Wheeler transform can also be computed in just linear time in the length of the text.

## The Inverse Burrows-Wheeler Transform

It is not obvious, but one of the most remarkable properties of the BWT is that it is invertible. Let's denote by $\text{BWT}^{-1}$ the inverse BWT, i.e. the transformation such that

$$\text{BWT}(\text{BWT}^{-1}(S)) = \text{BWT}^{-1}(\text{BWT}(S)) = S.$$

To prove that the BWT is invertible, let's first look at a very inefficient way of performing the inversion. Then, we will study a more efficient algorithm for the inverse BWT.

### The naive inversion method

The naive inversion algorithm reconstructs the entire BWT matrix $M$ starting from just the transformed string $\text{BWT}(S)$. For example, we will use our favourite string "banana$", whose BWT is given by "annb$aa". Initially, we know only the contents of the last column of $M$, since this contained the BWT string.

$$M = \begin{bmatrix} ? & ? & ? & ? & ? & ? & a \\ ? & ? & ? & ? & ? & ? & n \\ ? & ? & ? & ? & ? & ? & n \\ ? & ? & ? & ? & ? & ? & b \\ ? & ? & ? & ? & ? & ? & \$ \\ ? & ? & ? & ? & ? & ? & a \\ ? & ? & ? & ? & ? & ? & a \end{bmatrix}$$

Since the BWT matrix $M$ contains all of the cyclic permutations in sorted order, we know that in particular, the first column is sorted. Therefore, we can easily obtain the first column of $M$ by sorting the characters of BWT($S$). Sorting the characters of "annb$aa"gives "$aaabnn".

$$M = \begin{bmatrix} \$ & ? & ? & ? & ? & ? & a \\ a & ? & ? & ? & ? & ? & n \\ a & ? & ? & ? & ? & ? & n \\ a & ? & ? & ? & ? & ? & b \\ b & ? & ? & ? & ? & ? & \$ \\ n & ? & ? & ? & ? & ? & a \\ n & ? & ? & ? & ? & ? & a \end{bmatrix}$$

Next, we use the fact that we know that the last column of $M$ contains precisely the characters that precede the characters in the first column (Property 1). Therefore, if we append the first column of $M$ to the last column of $M$, we will obtain the set of all 2-mers of $S$ (length 2 substrings.) These 2-mers can then be sorted to obtain the first two columns the BWT matrix $M$.

$$\begin{bmatrix} a \\ n \\ n \\ b \\ \$ \\ a \\ a \end{bmatrix} + \begin{bmatrix} \$ \\ a \\ a \\ a \\ b \\ n \\ n \end{bmatrix} = \begin{bmatrix} a & \$ \\ n & a \\ n & a \\ b & a \\ \$ & b \\ a & n \\ a & n \end{bmatrix} \xrightarrow{\text{sort}} \begin{bmatrix} \$ & b \\ a & \$ \\ a & n \\ a & n \\ b & a \\ n & a \\ n & a \end{bmatrix}$$

So our reconstructed BWT matrix $M$ now looks like this.

$$M = \begin{bmatrix} \$ & b & ? & ? & ? & ? & a \\ a & \$ & ? & ? & ? & ? & n \\ a & n & ? & ? & ? & ? & n \\ a & n & ? & ? & ? & ? & b \\ b & a & ? & ? & ? & ? & \$ \\ n & a & ? & ? & ? & ? & a \\ n & a & ? & ? & ? & ? & a \end{bmatrix}$$

Again, we know that the final column of $M$ contains the characters that precede the characters in the first column (Property 1), so we can obtain the 3-mers (substrings of length 3) of $S$ by

appending the first two columns of $M$ to the final column. Sorting all of the 3-mers will then give us the first three columns of $M$.

$$\begin{bmatrix} a \\ n \\ n \\ b \\ \$ \\ a \\ a \end{bmatrix} + \begin{bmatrix} \$ & b \\ a & \$ \\ a & n \\ a & n \\ b & a \\ n & a \\ n & a \end{bmatrix} = \begin{bmatrix} a & \$ & b \\ n & a & \$ \\ n & a & n \\ b & a & n \\ \$ & b & a \\ a & n & a \\ a & n & a \end{bmatrix} \xrightarrow{\text{sort}} \begin{bmatrix} \$ & b & a \\ a & \$ & b \\ a & n & a \\ a & n & a \\ b & a & n \\ n & a & \$ \\ n & a & n \end{bmatrix}$$

We now just repeat this process until we have the entire matrix. Append the first $k$ columns to the final column and sort the results to obtain the first $k+1$ columns and repeat until we have reconstructed the entire matrix $M$. Once we have reconstructed the entire matrix, the original string $S$ is simply the row that ends with the \$ character, or equivalently, it is the first row cyclically shifted one character to the left.

$$M = \begin{bmatrix} \$ & b & a & n & a & n & a \\ a & \$ & b & a & n & a & n \\ a & n & a & \$ & b & a & n \\ a & n & a & n & a & \$ & b \\ \mathbf{b} & \mathbf{a} & \mathbf{n} & \mathbf{a} & \mathbf{n} & \mathbf{a} & \mathbf{\$} \\ n & a & \$ & b & a & n & a \\ n & a & n & a & \$ & b & a \end{bmatrix}$$

While this construction demonstrates that indeed the BWT can be inverted, it is not an efficient way of doing so. Some more clever observations about the properties of the BWT and the matrix $M$ will help us to derive a more efficient inversion algorithm.

## Efficient inversion of the BWT

The key to performing the inversion of the BWT fast is a single powerful observation called the **LF-mapping**.

**Property 5: The LF-mapping of the BWT matrix**

In the BWT matrix $M$, the $i^{\text{th}}$ occurrence of a character $C$ in the **last column (L)** corresponds to the $i^{\text{th}}$ occurrence of $C$ in the **first column (F)**.

In other words, the first occurrence of 'a' in the last column corresponds to the first occurrence of 'a' in the first column, the third occurrence of 'r' in the last column corresponds to the third occurrence of 'r' in the first column and so on.

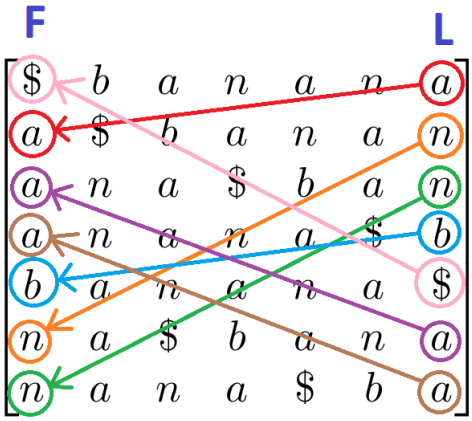



Figure 11.1: The LF-mapping for the BWT matrix $M$ of the string “banana$”

**Proof: Why the LF-mapping works**

Consider all of the occurrences of some character $C$ in the last column (L) of the BWT matrix. Since the characters of the last column precede the characters of the first column (Property 1), the relative sorted order of the occurrences of $C$ in the last column is decided by the lexicographical order of the corresponding rows, i.e. the suffixes succeeding the occurrences of $C$.

Since the rows of the matrix $M$ are sorted lexicographically, we find all occurrences of $C$ grouped together in the first column, which means they will be sorted by whatever succeeds them, i.e. the suffixes succeeding them. Therefore the occurrences of the character $C$ in the first column and the last column are both sorted by the suffixes succeeding them, hence they are sorted in the same relative order.

Utilising the LF-mapping, we can quickly and efficiently produce the inverse BWT of a string. Given the BWT of a string BWT($S[1..n]$), we will produce the original string one character at a time by starting from the end and following the LF-mapping to each previous character until we reach the end again. We know that the final character is always the special terminating character $ which occurs only once in the string, so we know our initial location in the last column is in the position at which ’$’ occurs.

Using the string “banana$” to demonstrate:

current_string = "$", current_position = 5

Since we are at the first occurrence of ’$’ in the string, using the LF-mapping, we know that the corresponding location in the first column would be the first occurrence of ’$’, which would occur at position 1. Invoking Property 1 yet again, we know that the previous character in the string must be the one at position 1 in the last column (the BWT string), which is an ’a’.

current_string = "$a", current_position = 1

Now we are at position 1, and since this is the first occurrence of the character 'a', we know that the corresponding position in the first column of $M$ will be the first occurrence of 'a' there, which is at position 2. Again, using Property 1, we can deduce that the next previous character in our reconstructed string is the one in position 2 of the BWT string, which is an 'n'.

$$\text{current\_string} = \text{"\$an"}, \qquad \text{current\_position} = 2$$

At position 2 we are looking at the first occurrence of 'n', so we calculate that the first occurrence of 'n' in the first column would be at position 6 (this can be computed by the fact that there are 5 characters in the string that are lexicographically less than 'n'). Using Property 1, we know that the previous character in the string is therefore 'a' (the $6^{\text{th}}$ character in the BWT string.)

$$\text{current\_string} = \text{"\$ana"}, \qquad \text{current\_position} = 6$$

We are at position 6 looking at the second occurrence of 'a', so we calculate that the second occurrence of 'a' occurs at position 3 in the first column, and hence deduce that the previous character in the string is an 'n'.

$$\text{current\_string} = \text{"\$anan"}, \qquad \text{current\_position} = 3$$

From position 3 at the second occurrence of 'n' in the last column, we find that the second occurrence of 'n' in the first column appears at position 7, so the previous character of the string is the one at position 7 in the transformed string, which is the third 'a'.

$$\text{current\_string} = \text{"\$anana"}, \qquad \text{current\_position} = 7$$

Finally, from the location of the third 'a', we calculate that the previous character is at position 4, which corresponds to a 'b' in the transformed string.

$$\text{current\_string} = \text{"\$ananab"}, \qquad \text{current\_position} = 4$$

If we followed the LF-mapping one more time, we would arrive back at the '$' character where we began. Now that we are finished, we can simply reverse the reconstructed string to obtain the inverted text "banana$". Notice how this entire process never uses any of the columns of the matrix $M$ except for the first and the last. This process is depicted in Figure 11.2

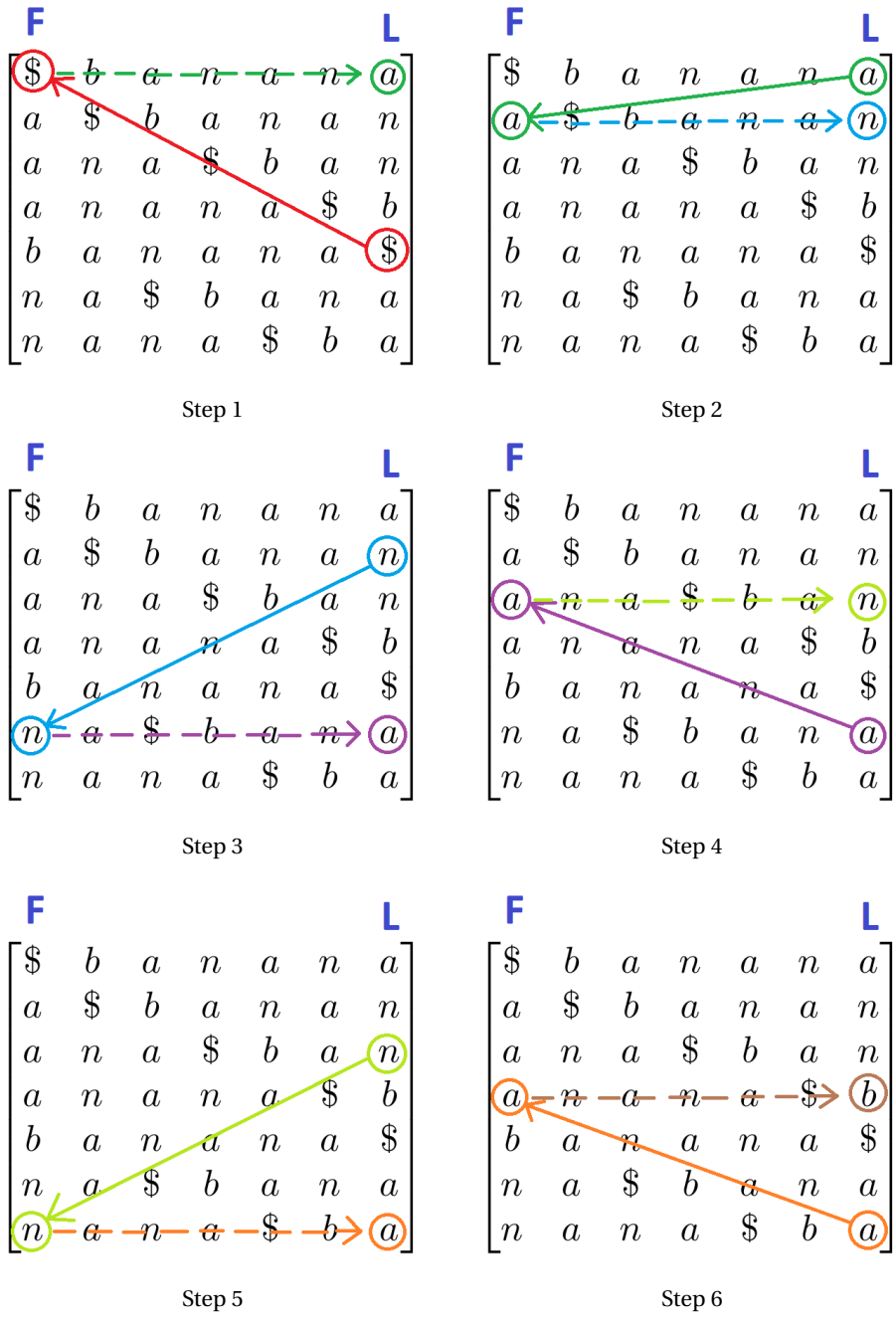



Figure 11.2: The LF-mapping applied to recover the string `banana$`

### Implementing the inversion algorithm

Next, we should figure out how to actually do this inversion quickly. Clearly if we just iterate through the transformed string at every step to find out which occurrence we are looking at, the entire process will take $O(n^2)$, which is still not very good. To avoid this, we make the following powerful observation. The LF-mapping can be computed by observing that the position of the character $c$ in row $i$ in the last row is given by the formula

$$\text{position} = \text{rank}(c) + \text{Occ}(c, i-1),$$

where $\text{rank}(c)$ is the position of the first $c$ in the left column, and $\text{Occ}(c, i)$ gives the number of occurrences of the character $c$ in the prefix $\text{bwt}[1..i]$. In other words, the corresponding position is simply the index of the first occurrence of $c$ plus 1 for each occurrence of $c$ that came before position $i$ in the transformed text. In order to compute this fast, we should pre-compute the ranks and the number of occurrences $\text{Occ}(c, i-1)$ for each position. This can be done as follows:

1. First, perform a linear pass over the transformed text and count the number of occurrences of each character. This is equivalent to performing the first half of the counting sort algorithm, where we compute the positions of the sorted elements.
2. At each position, before incrementing, save the current value of the counter for that character since it gives precisely the value $\text{Occ}(c, i-1)$.

This is all brought together and implemented in Algorithm 49. The pre-computation takes $O(n)$ time, and we take $O(n)$ steps to follow the LF-mapping, so the total running time is $O(n)$.

**Algorithm 49** Inverse Burrows-Wheeler transform

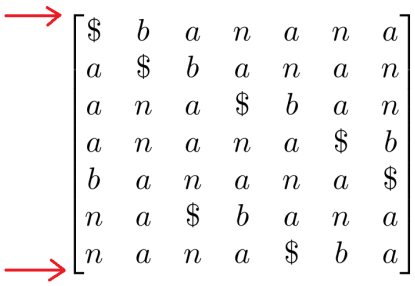
```
1:  function INVERSE_BWT(bwt[1..n])
2:      Set count[Σ] = 0
3:      Set rank[Σ] = 0
4:      Set occ[1..n] = 0        // occ[i] gives the value of Occ(bwt[i], i-1)
5:      for i = 1 to n do
6:          occ[i] = count[bwt[i]]
7:          count[bwt[i]] += 1
8:      end for
9:      Set location = 1
10:     for each character c in Σ do
11:         rank[c] = location
12:         location += count[c]
13:     end for
14:     Set S[1..n] = "$"
15:     Set pos = rank['$']
16:     for i = n − 1 to 1 do
17:         S[i] = bwt[pos]
18:         pos = rank[bwt[pos]] + occ[pos]
19:     end for
20:     return S[1..n]
21: end function
```

## Pattern Matching with the Burrows-Wheeler Transform

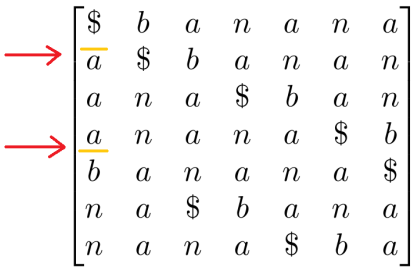
In its original inception, the Burrows-Wheeler transform was designed and implemented for the purposes of data compression. Many years later, it was discovered that transform's close similarities to the suffix array combined with the LF-mapping could actually be used to perform fast pattern matching on the original text. We have already seen how to perform pattern matching in just $O(m\log(n))$ or $O(m)$ with a suffix array or suffix tree respectively. BWT, like these two is highly applicable to situations where we have a single extremely large text string $T[1..n]$ and a large number of relatively small patterns $P[1..m]$.

Since the BWT matrix consists of the sorted cyclic shifts of the text $T$, as was the case for suffix arrays, all occurrences of a particular pattern will occur at indices that form a contiguous section of the sorted cyclic shifts. We exploit the LF-mapping to locate this range for each suffix of the pattern $P$. The algorithm searches the pattern string $P$ from the back, finding at each step, the range of locations of the cyclic shifts of $T$ that have the current suffix as a prefix. The suffix is expanded, adding an additional character at each step and finding the new matching locations fast by exploiting Property 1 and the LF-mapping.

Let's make this clear with an example. Consider our favourite text string "banana$" and suppose that we are searching for the pattern "ana". Initially, we consider the empty suffix of "ana", the empty string, so the entire matrix is a match (everything contains the empty string as a prefix).

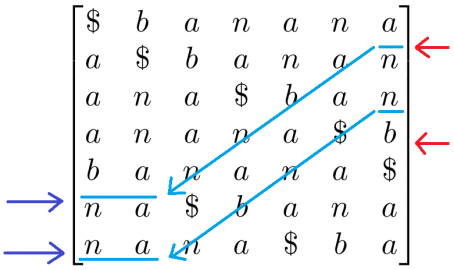


We begin searching from the back of "ana", so we first locate the cyclic shifts that contain "a" as a prefix, which corresponds to positions 2 - 4 in the BWT matrix.

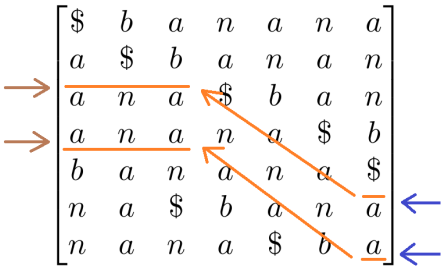


Now for the interesting part, we wish to expand the suffix 'a' to the suffix "na" and find all cor-

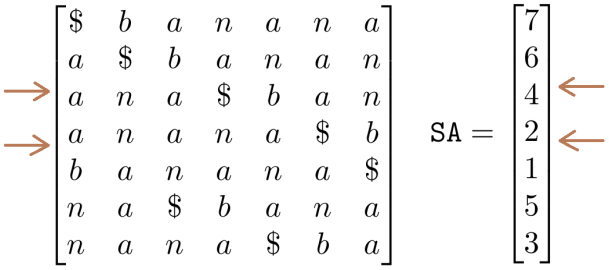
responding matches in the prefixes of the cyclic shifts of $T$. Using Property 1, we know that any 'n's that precede the 'a's that we are looking at can be found by looking at the final column. Inspecting the final column shows us that there are two 'n's within the current range, which we can locate using the LF-mapping.



The current matching range now points to the locations of the cyclic shifts that have "na" as a prefix. We want to expand the suffix "na" to become "ana" and find the new corresponding locations of the prefixes. Again, we use Property 1 and look in the last column for the occurrences of 'a' that lie within the current matching range. We see that the current matching range contains the second and third 'a', so we locate them in the first column using the LF-mapping.



The matching range now points to all cyclic shifts that contain "ana" as a prefix, which means we have found all occurrences of "ana" as a substring. Remember that we do not actually have the entire matrix in memory (it would take $O(n^2)$ memory to store), so to actually obtain the indices at which the matches occur, we would use the suffix array.



Looking in the suffix array at the range we just found, we see that the substring "ana" should occur at positions 4 and 2, which is correct.

## Implementing the pattern matching algorithm

Implementing this pattern search algorithm efficiently follows most of the same ideas as the inverse transform algorithm. We need to precompute the counts and rank of each character in the alphabet. Additionally, in order to perform the LF-mapping, we need to be able to compute $\text{Occ}(c, i)$ for all characters $c$ and positions $i$.

If we maintain the current matching range with two indices *start* and *end*, then we can observe that updating these pointers to account for the next character $P[i]$ in the pattern can be done in $O(1)$ using the LF-mapping by the following formulas:

$$\begin{cases} \text{start} = \text{rank}(P[i]) + \text{Occ}(P[i], \text{start} - 1) \\ \text{end} \ = \text{rank}(P[i]) + \text{Occ}(P[i], \text{end}) - 1 \end{cases}$$

Note that this is very similar to the inverse transformation. The simplest way to compute $\text{Occ}(c, i)$ is to precompute it for all characters $c$ and positions $i$. This will use $O(|\Sigma|n)$ space which is quite large, but will allow for the queries to be processed in $O(m)$. An algorithm computing these statistics is depicted in Algorithm 50.

**Algorithm 50** Computation of the BWT statistics

```
1:  function BWT_INDEX(bwt[1..n])
2:      Set count[Σ] = 0
3:      Set rank[Σ] = 0
4:      Set occ[Σ][1..n] = 0        // occ[c][i] gives the value of Occ(c,i)
5:      for i = 1 to n do
6:          count[bwt[i]] += 1
7:          for each character c in Σ do
8:              occ[c][i] = count[c]
9:          end for
10:     end for
11:     Set location = 1
12:     for each character c in Σ do
13:         rank[c] = location
14:         location += count[c]
15:     end for
16:     return rank, occ
17: end function
```

With everything precomputed, the pattern matching algorithm is very simple. An example implementation is given in Algorithm 51. The algorithm will return the range of matches [start, end], which can then be looked up in the suffix array if desired. If only the number of occurrences of the pattern is required and not their positions, then the suffix array is not necessary. If the range [start, end] is empty (i.e. start > end) then no matches were found. Since the precomputed statistics allow us to update the *start* and *end* pointers in $O(1)$ for each character of the pattern $P[1..m]$, the worst case time complexity of the pattern matching algorithm is $O(m)$.

**Algorithm 51** Pattern matching using the BWT

```
1: function FIND_PATTERN(P[1..m], rank[Σ], occ[Σ][1..n])
2:     Set start = 1, end = n
3:     for i = m to 1 do
4:         if start > end then break
5:         start = rank[P[i]] + occ[P[i]][start-1]
6:         end = rank[P[i]] + occ[P[i]][end] - 1
7:     end for
8:     return start, end
9: end function
```

Alternatively, a more memory conservative solution is to record the locations of each character and use binary search to compute $\text{Occ}(c, i)$ in $\log(n)$ time, which worsens the query time to $O(m \log(n))$ but drastically reduces the space usage.

It turns out that it is also possible to compute $\text{Occ}(c, i)$ in constant time using less than linear space by compressing the transformed string, splitting it into machine-word-sized substrings and applying clever bit tricks. This allows for optimal $O(m)$ query time and optimal space usage! This data structure is called the FM-index[1], but it is a bit advanced for us to cover right now.

[1] See Ferragina and Manzini, Opportunistic Data Structures with Applications, *FOCS* 2000

# Chapter 12

# Graph Traversal

Graphs are a simple way of modelling sets of objects and encoding relationships between those objects. Despite their simplicity on the surface, graphs have an enormous number of applications in a wide range of fields. Graph problems are ubiquitous not only in computer science, but in modelling complex processes and situations in all disciplines of science and business. We will begin our study of graphs with the two most fundamental ideas that we will need to absorb, which are representation: how do we actually model and store a graph, and traversal: how do we examine the contents of a graph to determine its underlying properties.

**Summary: Graph representation and traversal**

In this chapter, we cover:

- Modelling real-world problems with graphs and formal descriptions of graphs
- Representation and storage techniques for graphs
- Graph traversal algorithms with applications

**Recommended Resources: Graph representation and traversal**

- CLRS, Introduction to Algorithms, Sections 22.1, 22.2, 22.3
- Weiss, Data Structures and Algorithm Analysis, Section 12.4.1
- `https://visualgo.net/en/graphds` - Visualisation of graphs
- `https://visualgo.net/en/dfsbfs` - Visualisation of graph traversal
- `https://youtu.be/s-CYnVz-uh4` - MIT 6.006 lecture on breadth-first search
- `https://youtu.be/AfSk24UTFS8` - MIT 6.006 lecture on depth-first search
- `http://users.monash.edu/~lloyd/tildeAlgDS/Graph/`

## Modelling with Graphs

At the most basic level, graphs tell us about relationships between pairs of objects. Graphs that model objects with particular attributes are often referred to as *networks*, although the terms can usually be used interchangeably, so don't worry about the distinction. For example, consider a social network where friends connect with each other. We can represent this information

in a graph, where each person is represented by a *node* or *vertex* of the graph, and a connection between friends is denoted by an *edge* or *arc* connecting them. Given this graph, several interesting questions might immediately come to mind:

- What are the groups of mutual friends? i.e. friends that have a friend in common, or a friend-of-a-friend etc. (These are called the *connected components* of the graph)
- What is the largest degree of separation between two people in the network? (This would correspond to the longest *distance* between any people in the graph - also called its *diameter*)
- Are there any people in the network whom if removed would cause a pair of mutual friends to no longer be mutual friends? (Such a vertex in a graph is called an *articulation point* or *cut point*)

Graph and network algorithms can help us solve each of these problems.

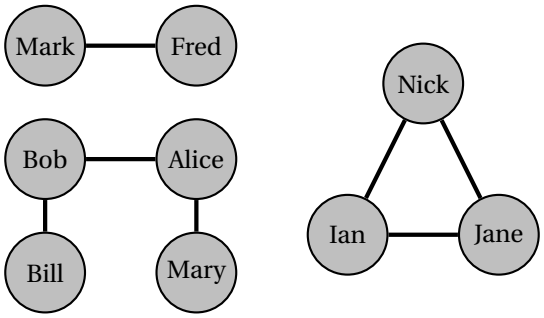



Figure 12.1: A network representing a set of people who have connections with each other.

Graphs can also be *weighted*. As another example, consider a road map of towns in the country, where each town is represented by a vertex, and roads between towns are represented by edges with *weights* corresponding to the distance between them.

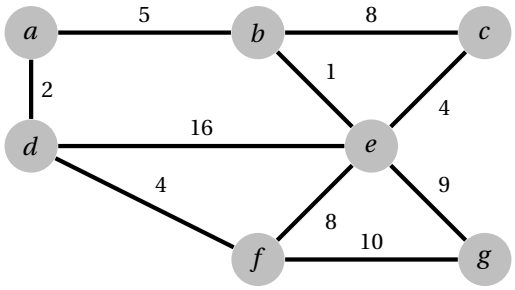



Figure 12.2: A network representing a road map of country towns.

Several interesting questions can be asked about such a graph:

- Given a pair of towns, what is the shortest route connecting them? (This is called the *shortest path problem*)

- What is the overall shortest subset of roads that we could keep, removing all others while still keeping every town connected? (This is called the *minimum spanning tree problem*)

Edges in a graph can also be directed, that is the relation only holds in one direction but not both. For example, consider your courses that you are taking for your degree, which have prerequisites that must be completed first. We can model this with a graph, in which a course has a directed edge to another course if the first course is a prerequisite of the second course and hence must be completed first.

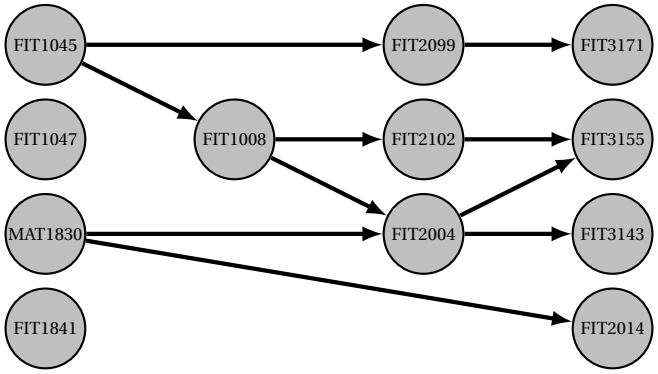



Figure 12.3: A network representing a course progression for a Computer Science degree.

Some more interesting questions now arise:

- Are there any cycles in the course graph? If so, the degree is impossible to complete! Ooops.
- If there aren't any cycles, what is a valid order to complete the courses in that satisfies all of the prerequisites? (Such an order is called a *topological ordering* of the graph.)
- If there aren't any cycles, what is the longest chain of prerequisites? i.e. assuming we could handle as many courses at a time as we wanted, how many semesters would it take us to complete the degree? (This is called the *critical path problem*)

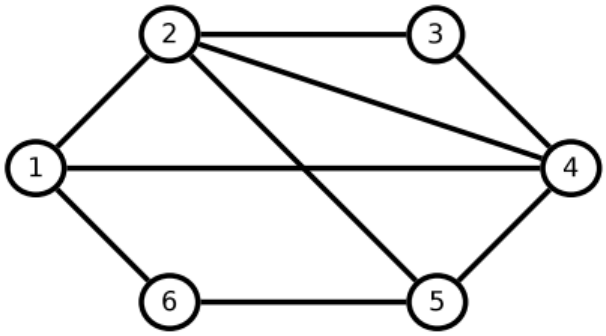
Once again, graph and network algorithms can help us solve all of these and many more problems!

## Formal graph notation

Formally, a graph $G$ is defined by a pair of sets $V$ and $E$, where

- $V$ is the the set of vertices / nodes.
- $E$ is the set of edges / arcs, where an edge $e$ connects two nodes $u$ and $v$

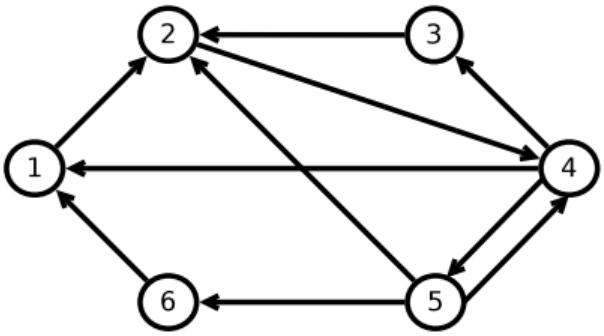
The number of vertices in a graph is usually either denoted by $|V|$, or as $n$ or $N$. Sometimes when the distinction is obvious and the writer is lazy, people will simply write $V$ to refer to the number of vertices. Similarly, we denote the number of edges by $|E|$, $m$ or $M$, or occasionally when being lazy and not totally accurate, by $E$.




An unweighted, undirected graph

**Direction**

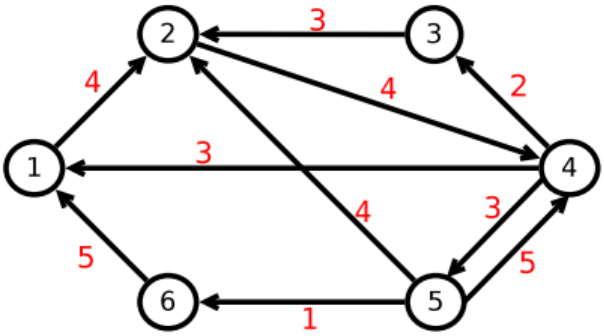
The edges of a graph may be *directed* or *undirected*. In an undirected graph, the edges $(u, v)$ and $(v, u)$ are equivalent, but in a directed graph, they represent different things (for example, a one-way street in a road map, or a course prerequisite, which are not the same if you reverse them!)




An unweighted, directed graph

**Weights**

The edges may also be *unweighted* or *weighted,* in which case they have an associated quantity, which may represent for example, the distance between two towns in a road map, the bandwidth of a connection in an internet network, the amount of money that it would cost to connect two houses via fibre-optic cable, or anything else you can imagine. We will usually denote the weight of the edge $(u, v)$ by $w(u, v)$.




A weighted, directed graph

#### Multigraphs and loops

Depending on the particular problem, it may be allowed or disallowed for a graph to contain multiple edges between the same pair of vertices. A graph that does contain multiple edges between the same pair of vertices is usually referred to as a *multigraph*.

Similarly, for a particular purpose, a graph may or may not be allowed to contain edges that connect a vertex to itself. Such edges are usually referred to as *loops*. A graph that contains no loops or multiple edges between the same pair of vertices is called a *simple graph*. If we do not specify otherwise, we will assume that the graphs we consider in this unit are simple by default.

## Representation and Storage of Graphs

There are several options that we may choose from when it comes to actually storing a graph for use in a computer program. The choice that we make will depend on the particular variety of graph and on the problem that we plan on solving.

### Considerations - Density of the graph

The biggest factor that will influence our decision of how to store our graph will be its *density*, which informally means does it have few edges or lots of edges. If we allow multiple edges between vertices, our graph can have an unbounded number of edges, so assume for now that our graphs do not have multiple edges.

- In a directed graph, the maximum number of possible edges that we can have is therefore $|V|^2$ if we allow loops, or $|V|(|V|-1)$ otherwise.
- In an undirected graph, the maximum number of possible edges is $\binom{|V|+1}{2}$ if we allow loops, or $\binom{|V|}{2}$ otherwise.

We say that a graph is *dense* if $|E| \approx |V|^2$, that is informally, the graph has a lot of edges. Conversely, we call a graph *sparse* if $|E| \ll |V|^2$, i.e. the graph has a relatively small number of edges.

## Representation strategy – Adjacency Matrix

One way to represent a graph is using an *adjacency matrix*. The adjacency matrix of a graph $G = (V, E)$ is a matrix $A$ of size $|V| \times |V|$. The space requirement of storing an adjacency matrix is therefore $O(|V|^2)$. When the edges are unweighted, the entries of the adjacency matrix are defined by

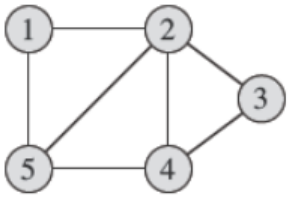
$$a_{i,j} = \begin{cases} 1, & \text{if there is an edge } (i,j) \\ 0, & \text{otherwise} \end{cases}.$$

In the case of multigraphs, adjacency matrices can be generalised such that $a_{i,j} = k$ where $k$ is the number of edges between vertices $i$ and $j$.

In a weighted graph, the adjacency matrix stores the weights of the edges, such that

$$a_{i,j} = \begin{cases} w(i,j), & \text{if there is an edge } (i,j) \\ 0 \text{ or } \infty, & \text{otherwise} \end{cases}.$$

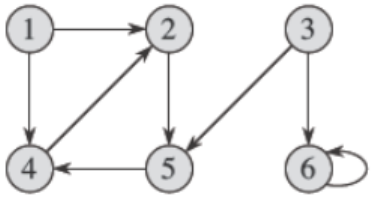
The choice of whether to use 0 or $\infty$ as an indicator that a particular edge is absent will depend completely on the problem at hand. The choice must be made such that the inclusion of the absent edge with the given weight does not change the solution to the problem being considered. Alternatively, if this is not feasible, one could store two matrices, one indicating adjacency without weights, and one storing the weights.




| | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| 1 | 0 | 1 | 0 | 0 | 1 |
| 2 | 1 | 0 | 1 | 1 | 1 |
| 3 | 0 | 1 | 0 | 1 | 0 |
| 4 | 0 | 1 | 1 | 0 | 1 |
| 5 | 1 | 1 | 0 | 1 | 0 |

An example of an adjacency matrix for an unweighted, undirected graph. Source: CLRS

In an undirected graph, the adjacency matrix will clearly be symmetric, so if we wish to, we can save memory by only storing the upper triangular entries. Given an adjacency matrix, checking whether two vertices have an edge between them can be done in constant $O(1)$ time by simply checking the corresponding entry in the adjacency matrix.

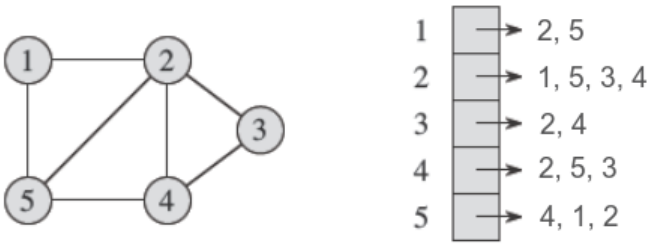



| | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 0 | 1 | 0 | 0 |
| 2 | 0 | 0 | 0 | 0 | 1 | 0 |
| 3 | 0 | 0 | 0 | 0 | 1 | 1 |
| 4 | 0 | 1 | 0 | 0 | 0 | 0 |
| 5 | 0 | 0 | 0 | 1 | 0 | 0 |
| 6 | 0 | 0 | 0 | 0 | 0 | 1 |

An example of an adjacency matrix for an unweighted, directed graph. Source: CLRS

## Representation strategy – Adjacency List

Adjacency matrices are good for representing dense graphs since they use a fixed amount of memory that is proportional to the total number of possible edges. However, when a graph is sparse, the corresponding adjacency matrix will contain a very large number of 0 entries, using the same $O(|V|^2)$ space regardless of the actual number of edges in the graph. In this case, a strong alternative is to store the graph in the form of an *adjacency list*. An adjacency list is simply a list of lists, where each list corresponding to a particular vertex stores the vertices that the given vertex is adjacent to. In a weighted graph, the adjacency list will store the weights of the edges alongside the vertices corresponding to those edges.




An example of an adjacency list for an unweighted, undirected graph. Source: CLRS

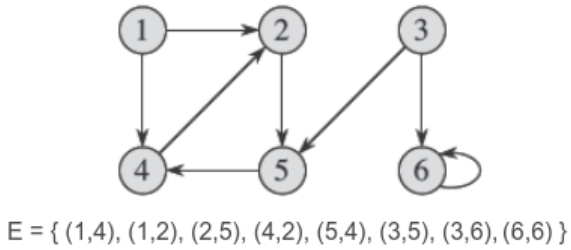
Since an adjacency list only uses memory for edges that actually exist in the graph, the space required for this representation is $O(|V|+|E|)$, which is a huge improvement over adjacency matrices for sparse graphs, and about the same for dense graphs.

Unlike with adjacency matrices, we can no longer check whether two given vertices are adjacent in constant time using an adjacency list. Adjacency lists are however, particularly convenient

when we only need to iterate over the existing edges since we will never need to examine a non-existent edge. We could instead store our adjacency list for each vertex in a balanced binary search tree, which would allow for $O(\log(|E|))$ adjacency checks while retaining the ability to iterate efficiently. Such a strategy would use more memory however and is not particularly useful for most applications.

### Representation strategy – Edge List

Although only rarely, sometimes we will opt for the *edge list* strategy. In this case, we simply store a list that contains all of the edges of the graph in no particular order.




An example of an edge list for an unweighted, directed graph. Source: CLRS

The edge list uses only $O(|E|)$ space, but affords us neither the ability to check adjacency quickly or iterate over the adjacent vertices of a particular vertex efficiently. Their primary use is in Kruskal's minimum spanning tree algorithm where we need to sort all of the edges in descending order of weight, which can not be done effectively with the other two representation strategies.

## Graph Traversal and Applications

A huge number of graph algorithms are built on a few small key ideas. The simplest and most wide reaching archetype of graph algorithm are the depth-first and breadth-first traversals. *Traversing* a graph simply means to explore it and figure out some of its properties.

### Depth-first search

A depth-first traversal as the name implies, searches a graph by following a path as deep as possible from some starting vertex before reaching a dead end, where there are no more adjacent and unvisited vertices, then backtracking up the path, continuing the search for vertices that have yet to be explored. In a depth-first traversal, we maintain a flag on each node that indicates whether or not we have visited that node yet. When a node is visited, we mark its flag as such in order to avoid visiting the same node multiple times and causing infinite repetition. An example graph is shown in Figure 12.4, with its vertices labelled in the order that a depth-first

search might visit them when starting from node $s$. We note that depth-first search always visits every node that is reachable from the source vertex, and since it can not visit a node twice, it never creates any cycles in its path. This implies that the edges travelled by the search form a tree, which we call a *depth-first search tree*.

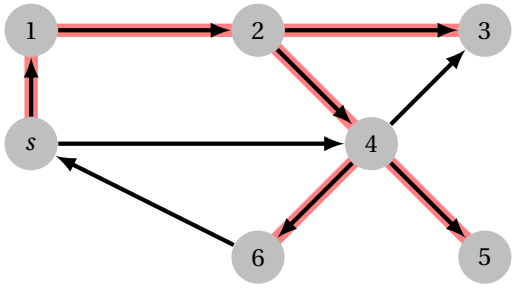



Figure 12.4: A graph with it's nodes labelled in the order that they might be visited by a depth-first search. The highlighted edges are those traversed by the search, forming a depth-first search tree

Depth-first search can be implemented very succinctly using recursion. We will assume that the graph is represented as an adjacency list, so that we can access adjacent vertices in constant time. A depth-first search is shown in Algorithm 52. Note that since the graph might not be connected, we loop over all vertices and make a call to DFS if that vertex has not been visited. Otherwise we may only visit one component of the graph (although for some applications, this may be all that is needed). This algorithm is applicable to both directed and undirected graphs.

**Algorithm 52** Generic depth-first search

```
1:  // Driver function that calls DFS until everything has been visited
2:  function TRAVERSE(G = (V, E))
3:      Set visited[1..n] = False
4:      for each vertex u = 1 to n do
5:          if not visited[u] then
6:              DFS(u)
7:          end if
8:      end for
9:  end function
10:
11: function DFS(u)
12:     visited[u] = True
13:     for each vertex v adjacent to u do
14:         if not visited[v] then
15:             DFS(v)
16:         end if
17:     end for
18: end function
```

We make the following assumptions to simplify the code:

1. Vertices are interchangeable with their ID number. That is, we will frequently loop over all vertices by looping over $1..n$, and we will read from and assign to arrays using vertices as indices.
2. Properties of the graph, for example the adjacency list, are visible to the DFS function. This avoids us having to pass around lots of extra arguments.
3. Quantities associated with the graph that we are working on are visible to the DFS function. For example, we assume that the DFS function can see and use the visited array even though it was declared in a different scope. This too saves on passing extra arguments around.

Since the depth-first search algorithm visits every vertex only once and examines every edge at most once (or twice for an undirected graph), its time complexity is $O(|V|+|E|)$. Despite its simplicity, the skeleton DFS algorithm forms the basis of a huge number of graph algorithms with wide-ranging applications. We will now explore a few of these applications.

#### Some applications of depth-first search

- Finding the connected components of a graph – the connected components of a graph are the maximal connected subgraphs, that is, they are the subsets of vertices that are mutually connected, directly or indirectly.
- Two-colouring a graph, or deciding that the graph can not be two-coloured – a graph can be two-coloured if every vertex can be assigned a colour, white or black, such that no two neighbouring vertices share the same colour. This is equivalent to the graph being bipartite.
- Finding a cycle in a graph – a cycle is a path consisting of a non-empty sequence of distinct, adjacent edges that begins and ends at the same vertex.
- Finding a topological ordering of a directed, acyclic graph (DAG) – a topological ordering is an ordering of the vertices of DAG such that all vertices $v$ that are reachable from the vertex $u$ come after it in the topological ordering, in other words, they are orderings that satisfy prerequisite relationships.
- Finding bridges and cut-points of a graph – these are edges and vertices that if removed from the graph would disconnect some connected component. In a sense they are "non-redundant" connections.

## Finding connected components

One of the simplest and most useful applications of graph traversal and depth-first search is finding the *connected components* of an undirected graph. The connected components of an undirected graph are the maximal connected subgraphs, that is, they are the subsets of vertices that are mutually connected, directly or indirectly.

We can find the connected components by observing that a single call to the depth-first search function visits precisely the connected component of the starting vertex, and nothing else. So

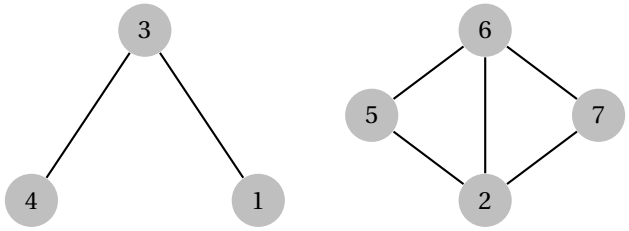



Figure 12.5: An unweighted, undirected graph with two connected components

we can simply run a depth-first search from each vertex that has not yet been visited by a previous one, and each time, we will discover one more component of the graph. An implementation is shown in Algorithm 53. Since the depth-first search runs in $O(|V|+|E|)$ time, this algorithm for determining the connected components also runs in $O(|V|+|E|)$.

**Algorithm 53** Finding connected components using depth-first search

```
1:  // Driver function that finds each connected component
2:  function CONNECTED_COMPONENTS(G = (V, E))
3:      Set component[1..n] = null
4:      Set num_components = 0
5:      for each vertex u = 1 to n do
6:          if component[u] == null then
7:              num_components += 1
8:              DFS(u, num_components)
9:          end if
10:     end for
11:     return num_components, component[1..n]
12: end function
13:
14: // One DFS will visit a single connected component
15: function DFS(u, comp_num)
16:     component[u] = comp_num
17:     for each vertex v adjacent to u do
18:         if component[v] == null then
19:             DFS(v, comp_num)
20:         end if
21:     end for
22: end function
```

After running CONNECTED_COMPONENTS, num_components will contain the number of connected components, each of which is identified by an integer from 1 to num_components. Each vertex $u \in V$ will have the ID number of the connected component that contains it stored in component[u]. Note that we do not need an explicit visited array, since we know whether or not a vertex has been visited by whether it has been assigned a component number yet. It is very common in depth-first search algorithms for the visited array to become redundant like this.

## Cycle-finding

Another useful application of depth-first search is locating cycles in graphs. Recall that a cycle is a path consisting of a non-empty sequence of distinct, adjacent edges that begins and ends at the same vertex. Consider an undirected, unweighted graph $G = (V, E)$. Suppose without loss of generality that $G$ is connected. Performing a depth-first search on $G$ will form a depth-first search tree $T$ that covers every vertex $v \in V$. If at any point the search finds an edge that leads to a vertex that it has already visited, then this edge connects two vertices $u, v$ that are already connected in $T$ and hence forms part of a cycle. We must be careful not to accidentally interpret the edge we just came from as a cycle though (since this "cycle" would use the same edge twice). To account for this, we'll have our DFS keep an extra parameter $p$, the vertex that we just came from, so that we know not to interpret $(u, p)$ as part of a cycle. Putting all of this together, an algorithm to find cycles in undirected graphs is shown in Algorithm 54.

**Algorithm 54** Cycle detection in an undirected graph using depth-first search

```
1:  // Driver function that calls DFS to look for a cycle
2:  function HAS_CYCLE(G = (V, E))
3:      Set visited[1..n] = False
4:      for each vertex u = 1 to n do
5:          if not visited[u] and DFS(u, null) = True then
6:              return True
7:          end if
8:      end for
9:      return False
10: end function
11:
12: // Returns True if a cycle was detected
13: function DFS(u, p)
14:     visited[u] = True
15:     for each vertex v adjacent to u do
16:         if visited[v] and v ≠ p then        // We found a cycle!
17:             return True
18:         else if DFS(v, u) = True then
19:             return True
20:         end if
21:     end for
22:     return False
23: end function
```

## Breadth-first search

Breadth-first search, like depth-first search traverses a graph one vertex at a time, never visiting a vertex more than once, until all reachable vertices have been visited. The only difference between the two is the order in which the vertices are visited. Many problems that can be solved with a depth-first search can also be solved with a breadth-first search. While a depth-first search explores paths as deep as possible immediately, a breadth-first search visits nearby

vertices first and further away vertices later. Formally, breadth-first search always visits every vertex that is a distance $k$ from the starting point before visiting any vertices that are a distance $k+1$. Like depth-first search, breadth-first search also produces a tree, but a much more special tree. Specifically, the tree produced by breadth-first search is a *shortest path tree*, a tree in which every path from the source $s$ is a shortest path in the original graph.

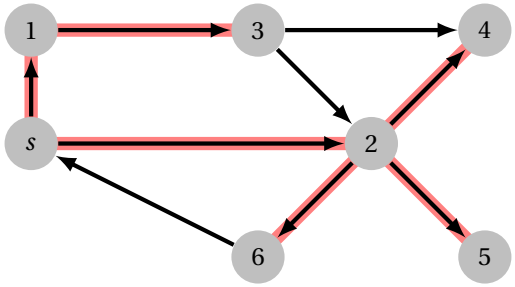



Figure 12.6: A graph with it's nodes labelled in the order that they might be visited by a breadth-first search. The traversed edges form a shortest path tree from $s$. Observe that all paths from $s$ in the tree use the fewest edges possible to reach their respective destinations.

Typically we use breadth-first search to explore a graph that is assumed to be connected, and hence we do not initiate multiple searches like we did in the depth-first search. This is completely a matter of convention. You can perform breadth-first search from multiple components if you want, and you may even search from multiple starting locations simultaneously. An implementation of breadth-first search is shown in Algorithm 55.

**Algorithm 55** Generic breadth-first search

```
1:  function BFS(G = (V, E), s)
2:      Set visited[1..n] = False
3:      visited[s] = True
4:      Set queue = Queue()
5:      queue.push(s)
6:      while queue is not empty do
7:          u = queue.pop()
8:          for each vertex v adjacent to u do
9:              if not visited[v] then
10:                 visited[v] = True
11:                 queue.push(v)
12:             end if
13:         end for
14:     end while
15: end function
```

In order to visit vertices that are nearby sooner, the algorithm maintains a queue of vertices that need to be visited, appending progressively further vertices to the end of the queue as it traverses. Finally, note that just like the depth-first search, breadth-first search also visits each vertex at most once and examines each edge at most once (or twice for an undirected graph), hence its time complexity is $O(|V|+|E|)$.

### Unweighted shortest paths

Due to the fact that it visits vertices in distance order, breadth-first search can be used for finding the shortest paths in an unweighted graph from a given starting vertex s. We will track information about shortest paths by maintaining two arrays, dist[1..$n$] and pred[1..$n$], where dist[u] denotes the distance of the vertex u from our starting vertex s, and pred[u] denotes the vertex that proceeded u on the shortest path from s (the edge that the breadth-first search tree used to get to $u$). By maintaining these two arrays, we will be able to reconstruct the shortest paths from s to every other vertex. An implementation is illustrated in Algorithm 56.

**Algorithm 56** Single-source shortest paths in an unweighted graph

```
1:  function BFS(G = (V, E), s)
2:      Set dist[1..n] = ∞
3:      Set pred[1..n] = null
4:      Set queue = Queue()
5:      queue.push(s)
6:      dist[s] = 0
7:      while queue is not empty do
8:          u = queue.pop()
9:          for each vertex v adjacent to u do
10:             if dist[v] == ∞ then
11:                 dist[v] = dist[u] + 1
12:                 pred[v] = u
13:                 queue.push(v)
14:             end if
15:         end for
16:     end while
17: end function
```

Note that this algorithm does not only compute the shortest path between one pair of vertices, it computes the shortest paths from the source vertex s to **every other** reachable vertex in the graph. Once we have the shortest path information, we can reconstruct the sequence of vertices that make up the shortest path from s to the vertex u by backtracking through the pred array until we reach s. An implementation is depicted in Algorithm 57.

**Algorithm 57** Reconstruct shortest path

```
1:  function GET_PATH(s, u, pred[1..n])
2:      Set path = [u]
3:      while u ≠ s do
4:          path.append(pred[u])
5:          u = pred[u]
6:      end while
7:      return reverse(path)
8:  end function
```

# Chapter 13

# Shortest Paths

In this section, we will study the **shortest path** problem. Shortest paths are one of the most natural and useful graph problems that you will encounter. If you've ever used Google maps to find your way to a destination, then you've seen shortest paths problems in action. We have already seen a simple example of shortest paths, which were shortest paths on an unweighted graph, which could be determined as a by-product of a breadth-first search. Now we will explore more general shortest path algorithms for weighted graphs.

**Summary: Shortest paths**

In this chapter, we cover:

- Properties of shortest paths
- The single-source shortest path problem
- The Bellman-Ford algorithm
- Dijkstra's algorithm
- The all-pairs shortest path problem
- The Floyd-Warshall algorithm and its relation to the transitive closure problem

**Recommended Resources: Shortest paths**

- CLRS, Introduction to Algorithms, Chapter 24 and Section 25.2
- Weiss, Data Structures and Algorithm Analysis, Section 9.3
- `https://visualgo.net/en/sssp` - Visualisation of shortest paths
- `https://youtu.be/Aa2sqUhIn-E` - MIT 6.006 lecture on shortest paths
- `https://youtu.be/2E7MmKv0Y24` - MIT 6.006 lecture on Dijkstra'a algorithm
- `https://youtu.be/ozsuci5pIso` - MIT 6.006 lecture on Bellman-Ford
- `http://users.monash.edu/~lloyd/tildeAlgDS/Graph/Directed/`

## Definitions of Shortest Paths

The notion of a shortest path is intuitive, and may be stated informally as a path between vertices of a graph that minimises the total weight of the edges used in the path. One of the most obvious examples would be the idea of finding the shortest route on a road map from one location to another, in which we must decide which roads to take in order to minimise either the total distance travelled, or the time taken, or indeed any other quantity that we are interested in, such as toll costs. Note that we usually refer to **a** shortest path rather than **the** shortest path since there may be multiple equally short paths between two vertices.

Throughout this chapter, we will assume that we are dealing only with directed graphs. For graphs with nonnegative weights, this is no restriction since we can transform an undirected graph into a directed graph by replacing each edge $e = (u, v)$ with a pair of edges $e_1 = (u, v)$ and $e_2 = (v, u)$ of the same weight. It should be clear that shortest paths are unaffected by this transformation. For undirected graphs with negative weights however, things get more tricky, so we will not consider this case for now.

## Properties of Shortest Paths

Before diving straight in to the algorithms, we'll first take a look at some useful properties that shortest paths have which will help us in understanding the algorithms and how they work.

#### Shortest paths have optimal sub-structure

The first and most important observation that we can make about shortest paths is that they contain massive amounts of sub-structure. Consider the graph in the figure below. We can see that the shortest path from $1 \rightsquigarrow 7$ is through vertices $1 \to 2 \to 4 \to 7$ with a total weight of 6. Given that this is true, we know for sure that a shortest path from vertex 1 to vertex 4 must be $1 \to 2 \to 4$. Why? Since $1 \to 2 \to 4$ is part of the shortest path from $1 \rightsquigarrow 7$ (it is a *sub-path*), if it were not itself a shortest path, then we could replace this part of the original path with a shorter one, making our supposed shortest path even shorter. (Think about how you would prove this formally. **Hint:** Use contradiction.)

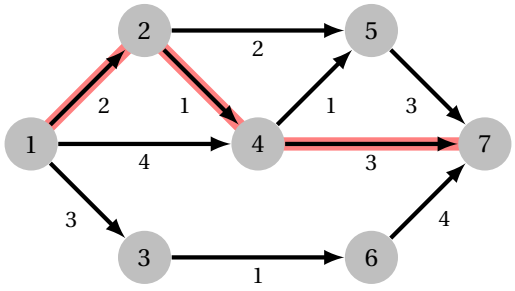



Figure 13.1: An weighted, directed graph. A shortest path from vertex 1 to vertex 7 has a total weight of 6, passing through the vertices $1 \to 2 \to 4 \to 7$.

#### Shortest paths satisfy the "triangle inequality"

Let us denote by $\delta(s,v)$ the length of a shortest path from vertex $s$ to vertex $v$. The triangle inequality says that for any edge $(u,v) \in E$ with weight $w(u,v)$, it is true that

$$\delta(s,v) \leq \delta(s,u) + w(u,v).$$

Behind these fancy symbols is a simple and intuitive but very critical fact that underpins most shortest path algorithms. All that this says in plain English is that if we have a shortest path $s \rightsquigarrow v$, then we can't find a path $s \rightsquigarrow u$, followed by an edge $u \rightarrow v$ with a shorter overall length, because this would mean that $s \rightsquigarrow u \rightarrow v$ would be an even shorter path. Expressed even more simply, you can't find a path that is shorter than your shortest path!

Why is this true? If the shortest path from vertex $s$ to vertex $u$ has total length $\delta(s,u)$ and the edge $(u,v)$ has weight $w(u,v)$ then we can form a path to vertex $v$ by taking a shortest path from $s$ to $u$ and then traversing the edge $(u,v)$, forming a path from $s$ to $v$. The total length of this path is $\delta(s,u) + w(u,v)$, so this length can not be shorter than the length of the shortest path, since it is itself a valid path. Try to formalise this argument using contradiction.

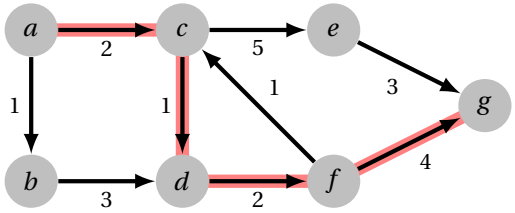



Figure 13.2: A weighted, directed graph. A shortest path from vertex $a$ to vertex $f$ has length 9. $\delta(a,e) = 7$, so the triangle inequality tells us that $\delta(a,f) \leq \delta(a,e) + w(e,f) = 7+3 = 10$, which is indeed satisfied. Since the bound is not tight, i.e. $\delta(a,f) < \delta(a,e) + w(e,f)$, this implies that the edge $(e,f)$ is not part of a shortest path from $a$ to $f$.

#### We can disregard cycles

Consider a path that contains a cycle in it. If this cycle has a positive total weight, then we can remove it from the path and the total weight decreases, so this path was not a shortest path. If the cycle has a negative total weight, then we may travel around the cycle over and over for as long as we wish and accumulate arbitrarily short paths, so the notion of a shortest path is not well defined in this case. Finally, if the path contains a cycle of zero total weight, then we may remove it and obtain a path with the same total weight. Therefore without loss of generality, we may assume that shortest paths are simple paths (contain no cycles) when looking for them.

For further details and proofs of shortest path properties, see CLRS Chapter 24.

## Shortest Path Problem Variants

There are three main variants of the shortest path problems that we might wish to consider.

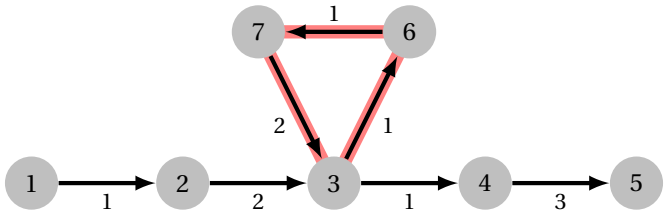



Figure 13.3: An edge weighted, directed graph containing a directed cycle. The cycle can not possibly be a part of a shortest path since it only makes the path length longer without going anywhere!.

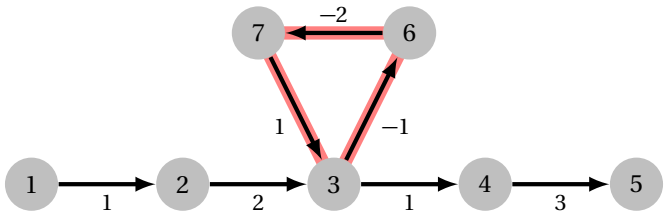



Figure 13.4: An edge weighted, directed graph containing a directed cycle with a negative total weight. The shortest path between vertex 1 and 5 is now **undefined**. For any path that you give me, I can always make an even shorter one by adding in another traversal of the cycle.

**Problem Statement: The single-pair shortest path problem**

Given a weighted, directed graph $G = (V, E)$ and a pair of vertices $u, v \in V$, find a shortest path between $u$ and $v$. Formally, find a sequence of adjacent vertices $(v_1, v_2, ..., v_k)$ such that the sum

$$\sum_{i=1}^{k-1} w(v_i, v_{i+1})$$

is minimised. In an unweighted graph, we consider $w(u, v) \equiv 1$, which is equivalent to asking for a path from $u$ to $v$ containing the fewest possible edges.

Although single-pair is seemingly the simplest possible shortest path problem, it turns out that the more general variants are typically simpler and asymptotically no more difficult to solve.

**Problem Statement: The single-source shortest path problem**

Given a weighted, directed graph $G = (V, E)$ and a starting vertex $s \in V$, find for every vertex $v \in V$ a shortest path from $s$ to $v$.

Given the copious amounts of substructure that is present in shortest paths, it should be intuitive that we can solve the single-source problem much faster than we could solve a single-pair problem separately for every possible vertex $v$.

**Problem Statement: The all-pairs shortest path problem**

Given a weighted, directed graph $G = (V, E)$, find a shortest path between every pair of vertices $u, v \in V$.

There is much overlap between these problems, and indeed each of them can be used to solve the former one. We will only explore algorithms for the last two of them since in general, it is usually the same difficulty to solve the first problem as the second, except in some special cases.

## Distance estimates and the relaxation technique

Most of the algorithms that we will study for shortest paths hinge on the technique of **relaxation**. For each of these algorithms, we are going to maintain a *distance estimate* for each vertex. That is, we will maintain for each vertex, the length of the shortest path to that vertex that we have found so far. Throughout the algorithms, we will continuously update these estimates and improve them as we find better paths. The notion of *relaxation* simply means to update a current shortest path to an even shorter path found by **enforcing the triangle inequality.** In other words, if we find an edge that violates the triangle inequality, then it means that we have found a path that is shorter than one of our current estimates, so we should update our estimate to the newer, shorter path. Edge relaxation is depicted in Algorithm 58 in Chapter 12.

**Algorithm 58** Edge relaxation

```
1: function RELAX(e = (u, v))
2:     if dist[v] > dist[u] + w(u, v) then
3:         dist[v] = dist[u] + w(u, v)
4:         pred[v] = u
5:     end if
6: end function
```

The predecessor array, just like in breadth-first search indicates for each vertex, its parent in the shortest path tree from the source. It is maintained in the same way as it was in a breadth-first search and can be used in the same way to reconstruct the shortest paths once we have found all of the correct distances (see Algorithm 57).

A very simple algorithm for finding single-source shortest paths would then be to simply relax all of the edges of the graph over and over until all of them satisfy the triangle inequality. Once the triangle inequality is satisfied for all of our distance estimates, then we know that our estimates are correct and we have all of the true shortest paths. This is in fact the basis of a shortest path algorithm called *Bellman-Ford.*

## The Bellman-Ford Algorithm

The Bellman-Ford algorithm is arguably the simplest algorithm for solving the single-source shortest paths problem in a weighted graph. Simply put, the Bellman-Ford algorithm repeat-

edly relaxes all of the edges of the graph until all of the shortest paths are obtained. More specifically, we relax every edge of the graph $|V|-1$ times. The reason for this will become clear shortly. A simple implementation is shown in Algorithm 59. The time complexity of Bellman-Ford is easy to establish: the outer loop runs for $|V|-1$ iterations, the inner loop runs for $|E|$ iterations, and each relaxation takes $O(1)$, so the total time taken is $O(|V||E|)$. Why do we need $|V|-1$ iterations? Let's explore that next.

**Algorithm 59** Bellman-Ford

```
1:  function BELLMAN_FORD(G = (V, E), s)
2:      Set dist[1..n] = ∞
3:      Set pred[1..n] = null
4:      Set dist[s] = 0
5:      for k = 1 to n-1 do
6:          for each edge e in E do
7:              RELAX(e)
8:          end for
9:      end for
10:     return dist[1..n], pred[1..n]
11: end function
```

## Correctness of Bellman-Ford

The key to establishing the correctness of Bellman-Ford lies in a simple property about paths in graphs. We write a formal proof of correctness using induction.

**Theorem: Correctness of Bellman-Ford**

The Bellman-Ford algorithm terminates with the correct distance estimates to all vertices whose shortest path is well defined after at most $|V|-1$ iterations.

**Proof**

In a well defined shortest path, the number of edges on the path can not be greater than $|V|-1$, why? If a path contained more than $|V|-1$ edges, then it must visit some vertex multiple times and hence contain a cycle, which we know we from our discussion before that we can ignore. We claim that after $k$ iterations of the Bellman-Ford algorithm, that all valid shortest paths consisting of at most $k$ edges are correct.

We can prove this formally by induction on the number of edges in each shortest path. For the base case, we initialise dist[s] = 0, which is correct if there is no negative cycle containing $s$. Hence all valid shortest paths containing zero edges are correct.

Inductively, suppose that all valid shortest paths containing at most $k$ edges are correct after $k$ iterations. Let's argue that all valid shortest paths containing at most $k+1$ edges are correct after one more iteration. Consider some shortest path from $s \rightsquigarrow v$ consisting of at most $k+1$ edges. By the substructure of shortest paths, the sub-path $s \rightsquigarrow u$ con-

sisting all but the final edge $(u, v)$ is a shortest path, and by our inductive hypothesis, is correctly estimated at the current iteration of the algorithm. If the current distance estimate of $v$ is incorrect, it will be relaxed in this iteration by the edge $(u, v)$ and hence be made correct since $\delta(s, v) = \delta(s, u) + w(u, v) = \text{dist[u]} + w(u, v)$.

Hence by induction on the number of edges in the shortest paths, all valid shortest paths consisting of at most $k$ edges are correctly estimated after $k$ iterations. Therefore the Bellman-Ford algorithm terminates correctly after at most $|V| - 1$ iterations.

## Dealing with negative cycles

An important problem that needs to be addressed is how to deal with the existence of negative cycles. As mentioned earlier, the presence of a negative cycle may cause the shortest path to a particular vertex to become undefined since there may exist paths of arbitrarily short length. In this case, the algorithm above will terminate with an arbitrary distance estimate to those vertices. Detecting and dealing with such paths is actually quite easy though, we simply appeal once more to **the triangle inequality.**

If a subset of the distance estimates satisfy the triangle inequality, then they must be valid shortest paths, so we can keep them. We can then seek out the distance estimates that violate the triangle inequality and conclude that those are the vertices that must be reachable via a negative weight cycle, and mark them as such. One way to view this is as performing relaxation but relaxing the distance to $-\infty$. See Algorithm 60.

**Algorithm 60** Bellman-Ford: Handling negative cycles

```
1: function MARK_UNDEFINED_PATHS(G = (V, E))
2:     for k = 1 to n do
3:         for each edge e = (u, v) in E do
4:             if dist[u] + w(u, v) < dist[v] then
5:                 dist[v] = −∞
6:             end if
7:         end for
8:     end for
9: end function
```

After running this post-processing step, all of the distances given in the dist array will be:

1. $\infty$ if the vertex in question was never reached (it is not connected to the source $s$)
2. $-\infty$ if the vertex in question is reachable via a negative cycle and hence does not have a shortest path
3. The correct distance if the vertex has a well defined shortest path

Note that the pred array may contain cycles if there are negative cycles present, so do not attempt to reconstruct shortest paths to vertices whose distance is undefined!

### Optimising Bellman-Ford

There are some simple optimisations that can be made to Bellman-Ford that improve its running time:

1. During the iterations of the main $k$ loop, if no relaxations are successful, then the shortest paths have already been found and we can terminate early.
2. If such an early termination occurs, then we are guaranteed that no negatives cycles exist and hence can skip the post-processing step that checks for undefined shortest paths.
3. Rather than iterating over every single edge, we could instead maintain a queue of edges that need to be relaxed. If an edge is not successfully relaxed in one phase, then it clearly need not be relaxed in the next phase either unless its source vertex has its distance estimate improved. For sparse graphs, this improves the empirical average case complexity of the algorithm to just $O(|E|)$, although the worst-case behaviour is unfortunately still $O(|V||E|)$. This variant is often referred to as the "Shortest Path Faster Algorithm."

## Dijkstra's Algorithm

Although the Bellman-Ford algorithm can handle every kind of graph for the single-source shortest path problem, i.e. any graph that has well defined shortest paths, it is not very efficient in practice even with optimisations. *Dijkstra's algorithm* presents us with a useful trade-off. Dijkstra's algorithm, unlike the Bellman-Ford algorithm is no longer capable of handing negative edge weights, but it is significantly faster both theoretically and in practice. Dijkstra's algorithm is a good example of trading off generality for a significant performance increase, and is widely applicable since many graphs encountered in practice do not require negative edge weights.

**Key Ideas: Dijkstra's Algorithm**

1. If all edge weights are non-negative, i.e. $w(u,v) \geq 0$ for all edges $(u,v)$, then any sub-path $s \rightsquigarrow u$ of some longer path $s \rightsquigarrow v$ necessarily has a length that is no greater than the entire path. This is not true when negative weights appear, as a path may grow in number of edges but decrease in total length due to the negative weights.
2. This means that if we know the distance to all vertices $u \in S$ for some set $S$ and we relax all edges that leave $S$, then we cn guarantee that the distance estimate to the vertex $v \notin S$ with the minimum estimate $\delta(s,u) + w(u,v)$ is optimal. This is because even though we do not know the distances to any other vertex $v' \notin S$, none of them can provide a shorter path to $v$ since all edge weights are nonnegative and hence the paths can only get longer.
3. Dijkstra's algorithm therefore employs a **greedy** approach, a similar idea to breadth-first search, by visiting nodes in order of distance from the source

In a sense, Dijkstra's algorithm is very similar to breadth-first search. The primary difference is that because the edge weights are no longer all the same, we can not simply use an ordinary

queue to store the vertices that we need to visit, since a path consisting of many low weight edges may have a shorter length than a path of fewer large weight edges. Instead, Dijkstra's algorithm employs a priority queue to ensure that vertices are visited in the correct order of their distance from the source[1]. An implementation is given in Algorithm 61.

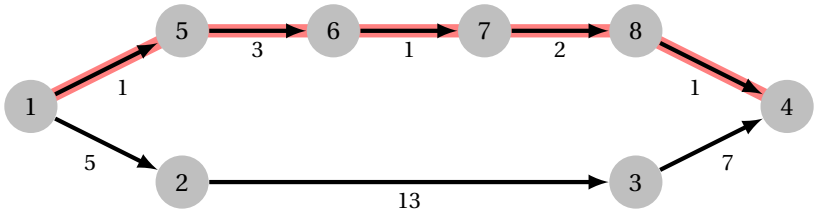



Figure 13.5: A graph where the shortest path from 1 ⇝ 4 has far more edges than the path with the fewest edges. In this case, breadth-first search can not be used to find shortest paths.

**Algorithm 61** Dijkstra's algorithm

```
1:  function DIJKSTRA(G = (V, E), s)
2:      Set dist[1..n] = ∞
3:      Set pred[1..n] = 0
4:      Set dist[s] = 0
5:      Set Q = priority_queue(V[1..n], key(v) = dist[v])
6:      while Q is not empty do
7:          u = Q.pop_min()
8:          for each edge e that is adjacent to u do
9:              // Priority queue keys must be updated if relax improves a distance estimate
10:             RELAX(e)
11:         end for
12:     end while
13:     return dist[1..n], pred[1..n]
14: end function
```

The priority queue Q is a minimum priority queue initially containing all vertices that serves each vertex $u$ in order of their current distance estimate dist[u]. At each iteration, the next vertex $u$ that has not been visited yet and which has the smallest current distance estimate is processed. Since vertices are removed in distance order, once a vertex has been removed from the queue, its distance estimate must be correct and will never be further modified.

## Complexity of Dijkstra's algorithm

The time complexity of Dijkstra's algorithm depends on the way in which we chose the implement the priority queue of vertices. In general, the time taken depends on two things, the amount of time required to find the next minimum, and the amount of time required to update

[1]Actually, Dijkstra's original implementation of his algorithm did not use a priority queue, but rather simply looped over the vertices to find which one was the next closest. This is very inefficient for sparse graphs however, and was improved by Fredman and Tarjan, who described the now standard min-heap-based priority queue implementation.

the distance estimates when we relax them. If we denote by $T_{\text{update}}$ and $T_{\text{find}}$, the time taken to update the distance estimates and to find the minimum respectively, then the total time complexity of Dijkstra's algorithm will be

$$O(|E| \cdot T_{\text{update}} + |V| \cdot T_{\text{find}}).$$

This is due to the fact that we relax every edge exactly once, performing an update operation each time in the worst-case, and we find and extract each vertex exactly once when it is the current minimum. If we implement Dijkstra's in the simplest way possible, using an array and looping over every vertex to find the minimum, then it takes constant $O(1)$ time to update the distances (we just update the dist array and nothing else) and linear $O(|V|)$ time to find the next vertex. Therefore the total running time would be

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

This can be improved significantly for sparse graphs by using a min-heap-based priority queue. If we use a standard binary heap data structure, we achieve $O(\log(|V|))$ time per operation for both find and update, and hence the time complexity of Dijkstra's algorithm becomes

$$O(|E|\log(|V|) + |V|\log(|V|)) = O(|E|\log(|V|)),$$

assuming the graph is connected. For dense graphs, this is actually slightly worse than the simple, array-based implementation, but for sparse graphs, this is a huge performance increase. Even better asymptotic complexities can be achieved by using fancier heap data structures such as the Fibonacci heap, but these often turn out to be less efficient in practice than their simpler counterparts.

## Correctness of Dijkstra's algorithm

We discussed the intuitive reasoning behind the correctness of Dijkstra's algorithm earlier. Since all edge weights are nonnegative, whenever we visit a closest vertex that hasn't been visited before, we can guarantee that no shorter path exists since any other paths we find can only be longer, since the only way to make a path shorter would be to add a negative weight somewhere. We prove this now formally using induction.

**Theorem: Correctness of Dijkstra's algorithm**

Given a graph $G = (V, E)$ with non-negative weights and a source vertex $s$, Dijkstra's algorithm correctly finds shortest paths to each vertex $v \in V$.

**Proof**

We can prove the correctness of Dijkstra's algorithm using a similar inductive argument to the one used for Bellman-Ford. Let's use induction on the set of vertices $S$ that have been removed from the queue, i.e. the set $S = V \setminus Q$. We will show for any vertex $v \in S$, that dist[v] is correct.

For the base case, we will always remove the source vertex $s$ first which has dist[s] = 0,

which is correct since the graph contains no negative weights.

Suppose for the purpose of induction that at some point it is true that for all $v \in S$, dist[v] is correct. Let $u$ be the next vertex removed from the priority queue, we will show that dist[u] must be correct.

Suppose for contradiction that there exists a shorter path for $s \rightsquigarrow u$ with a shorter distance $\delta(s \rightsquigarrow u) <$ dist[u]. Let $x$ be the furthest vertex along the correct $s \rightsquigarrow u$ path that is in $S$. Since $x \in S$, by the inductive hypothesis, its distance estimate is correct. Let $y$ be the next vertex on the shortest path after $x$. Since $\delta(s \rightsquigarrow u) <$ dist[u] **and all edge weights are non-negative**, it must be true that $\delta(s \rightsquigarrow y) \leq \delta(s \rightsquigarrow u) <$ dist[u]. But $y$ is adjacent to $x$ on a shortest path, which means the edge $(x, y)$ was relaxed when $x$ was removed from $Q$. This means that dist[y] $= \delta(s \rightsquigarrow y) <$ dist[u]. If dist[y] $<$ dist[u] and $y \neq u$, then Dijkstra's algorithm would have popped $y$ from the priority queue instead of $u$, a contradiction. Alternatively if $y = u$ and dist[y] $<$ dist[u], this is also a contradiction.

By contradiction, we conclude that dist[u] must be correct and hence by induction on the set $S$, when Dijkstra's algorithm terminates, dist[v] is correct for all $v \in V$.

Notice how the key step of the proof requires us to invoke the fact that the edge weights are non-negative. Without this restriction, this step of the proof would not be true, since the subpath $s \rightsquigarrow y$ might actually have a higher total weight than the total path $s \rightsquigarrow u$ due to negative weights later on.

## Practical considerations: Implementing Dijkstra's algorithm

When implementing Dijkstra's algorithm, careful thought needs to be put into the way in which the priority queue is going to be implemented. The most common description of the priority queue used for Dijkstra's algorithm is a min-heap that supports the following operations:

1. Insert the initial items into the priority queue,
2. Remove the item with the minimum key,
3. Decrease the key of an item already in the priority queue (whenever an edge is relaxed.)

In practice however, most programming language's standard library priority queues do not support operation 3, and implementing this operation ourselves can be annoying and tricky. An alternate formulation of Dijkstra's algorithm which does not require operation 3 is therefore commonly used instead. It works like this:

1. Begin with only the source vertex $s$ in the priority queue
2. Whenever an edge is relaxed, insert the target vertex in the priority queue keyed by its current distance estimate
3. When a key is removed from the priority queue, check whether it is out of date, and if so, ignore it. A key is out of date if key$(u) >$ dist$[u]$

The main idea here is that instead of updating the keys of vertices that are in the priority queue, we simply allow it to contain multiple entries for the same vertex with different distance esti-

mates. If a vertex $u$ that has already been processed is popped from the queue, the key will be greater than dist[$u$] and hence we can ignore it since it is an out-of-date entry. This does not hurt the asymptotic complexity of the algorithm, since the only difference encountered is that the priority queue may grow to a worst-case size of $|E|$ instead of $|V|$, leading to operations that cost $O(\log(|E|))$ instead of $O(\log(|V|))$. But since in a simple graph

$$O(\log(|E|)) = O(\log(|V|^2)) = O(2\log(|V|)) = O(\log(|V|)),$$

this is asymptotically equivalent (and we can always preprocess a graph to make it simple by taking just the shortest edge between every pair of vertices). In practice, the number of entries in the priority queue at any given time is likely to be much smaller than $|E|$, so this method is almost always a speed-up too, except in pathological cases. An example implementation is depicted in Algorithm 62.

**Algorithm 62** Improved Dijkstra's algorithm

```
1:  function DIJKSTRA(G = (V, E), s)
2:      Set dist[1..n] = ∞
3:      Set pred[1..n] = 0
4:      Set dist[s] = 0
5:      Set Q = priority_queue()
6:      Q.push(s, key = 0)
7:      while Q is not empty do
8:          u, key = Q.pop_min()
9:          if dist[u] < key then        // Do no process an out-of-date entry
10:             for each edge e that is adjacent to u do
11:                 if dist[v] > dist[u] + w(u, v) then
12:                     dist[v] = dist[u] + w(u, v)
13:                     pred[v] = u
14:                     Q.push(v, key = dist[v])
15:                 end if
16:             end for
17:         end if
18:     end while
19:     return dist[1..n], pred[1..n]
20: end function
```

## The All-Pairs Shortest Path Problem

Finally, we consider the all-pairs shortest path problem, in which we seek a shortest path between every pair of vertices in the given graph. The most obvious solution to this problem is to simply solve the single-source shortest path problem using every possible vertex as the source. This might sound inefficient, but for certain graphs this is actually the optimal solution.

- Consider an unweighted graph. If we perform a breadth-first search from every possible source, each taking $O(|V|+|E|)$ time, then the complexity of finding all-pairs shortest paths is $O(|V|(|V|+|E|))$.

- In graph with nonnegative weights, we can run Dijkstra from every possible source and achieve a runtime of $O(|V||E|\log(|V|))$ assuming that our priority queue is a binary heap.
- In a graph with negative weights, multiple invocations of Bellman-Ford from every source would yield a time complexity of $O(|V|^2|E|)$.
- (**Not examinable in Semester Two, 2018**) For graphs with negative weights, multiple invocations of Bellman Ford is extremely slow. However, a clever trick exists called the *potential method* that allows us to re-weight the graph in such a way that we get rid of all of the negative weight edges without changing the shortest paths. Multiple invocations of Dijkstra's algorithm can then be made on the modified graph before reverting the weights and recovering the shortest paths. This algorithm is called Johnson's algorithm and has a runtime of $O(|V||E|\log(|V|))$, assuming Dijkstra's is implemented with a binary heap.

## The Floyd-Warshall algorithm

The Floyd-Warshall algorithm is a very simple all-pairs shortest path algorithm that is fast for dense graphs, but can be beaten in performance on sparse graphs by multiple invocations of the single-source algorithms as described above. Floyd-Warshall relies on the observation that a shortest path from $u \rightsquigarrow v$ that has at least two edges can be decomposed into two shortest paths $u \rightsquigarrow k$ and $k \rightsquigarrow v$ for some intermediate vertex $k$. The algorithm simply iteratively increases the pool of intermediate vertices $k$ from 1 to $n$ and updates all paths that can be improved by visiting vertex $k$ as an intermediate step.

We initialise the all-pairs distance estimate as a 2D matrix dist[1..$n$][1..$n$] such that dist[v][v] = 0 for all vertices $v$ and dist[u][v] = $w(u,v)$ for all edges $e = (u,v)$. Observe that if the graph is represented as an adjacency matrix, then initialising the distance matrix dist is easy as this is nothing but a copy of the adjacency matrix! See the implementation in Algorithm 63. The time complexity of Floyd-Warshall is obvious. There are three loops from 1 to $n$ and a constant time update each iteration, so the total runtime is $O(|V|^3)$. The space complexity is $O(|V|^2)$ since we store the $|V| \times |V|$ dist matrix.

**Algorithm 63** Floyd-Warshall

```
1:  function FLOYD_WARSHALL(G = (V, E))
2:      Set dist[1..n][1..n] = ∞
3:      Set dist[v][v] = 0 for all vertices v
4:      Set dist[u][v] = w(u,v) for all edges e = (u,v) in E
5:      for each vertex k = 1 to n do
6:          for each vertex u = 1 to n do
7:              for each vertex v = 1 to n do
8:                  dist[u][v] = min(dist[u][v], dist[u][k] + dist[k][v])
9:              end for
10:         end for
11:     end for
12:     return dist[1..n][1..n]
13: end function
```

Comparing this against the running times of the repeated single-source solution, we can see

that for dense graphs, where $|E| \approx |V|^2$, Floyd-Warshall is the best or equal best in all cases. For sparse graphs however ($|E| \approx |V|$), Floyd-Warshall is beaten by $O(|V|^2)$ and $O(|V|^2 \log(|V|))$.

| | **Sparse** | **Dense** |
|---|---|---|
| **BFS** | $O(\|V\|^2)$ | $O(\|V\|^3)$ |
| **Dijkstra** | $O(\|V\|^2 \log(\|V\|))$ | $O(\|V\|^3 \log(\|V\|))$ |
| **Bellman-Ford** | $O(\|V\|^3)$ | $O(\|V\|^4)$ |
| **Johnson** (Not examinable) | $O(\|V\|^2 \log(\|V\|))$ | $O(\|V\|^3 \log(\|V\|))$ |
| **Floyd-Warshall** | $O(\|V\|^3)$ | $O(\|V\|^3)$ |

Finally, note that just like Bellman-Ford, Floyd-Warshall can handle negative weights just fine, and can also detect the presence of negative weight cycles. To detect negative weight cycles, simply inspect the diagonal entries of the dist matrix. If a vertex $v$ has dist[v][v] $< 0$, then it must be contained in a negative weight cycle.

## Correctness of Floyd-Warshall

**Theorem: Correctness of Floyd-Warshall**

Floyd-Warshall produces the correct distances for all pairs of vertices $(u, v)$ such that there exists a shortest path between $u$ and $v$.

**Proof**

We will establish the following invariant: After $k$ iterations of Floyd-Warshall, dist[u][v] contains the length of a shortest path $u \rightsquigarrow v$ consisting only of intermediate vertices from 1 to $k$.

For $k = 0$, we have performed no iterations yet. dist[u][v] is therefore equal to $w(u, v)$ if an edge exists between $u$ and $v$. Using no intermediate vertices at all, the is the only path possible, and hence it is the shortest path possible. If $u = v$, then dist[u][v] $= 0$ which is optimal using no other vertices. If there is no edge $(u, v)$, then dist[u][v] $= \infty$ which is correct since no paths are possible yet.

Suppose that after iteration $k$, dist[u][v] contains the length of a shortest path $u \rightsquigarrow v$ consisting only of intermediate vertices from 1 to $k$. We will show that after iteration $k+1$, dist[u][v] contains the length of a shortest path $u \rightsquigarrow v$ consisting only of intermediate vertices from 1 to $k+1$. Consider a shortest path between some vertices $u$ and $v$ consisting of intermediate vertices in 1 to $k+1$. If vertex $k+1$ is not a part of the path then by the inductive hypothesis we already have the optimal length. Otherwise, this path contains only one occurrence of vertex $k+1$, since if it contained multiple, it would contain a cycle. Therefore there exists two sub-paths $u \rightsquigarrow k+1$ and $k+1 \rightsquigarrow v$ which do not contain vertex $k+1$ as an intermediate vertex. By the inductive hypothe-

sis, dist[u][k+1] and dist[k+1][v] are optimal, and since together they form the shortest path, the update will set dist[u][v] = dist[u][k+1] + dist[k+1][v] which is now optimal. Therefore after iteration $k+1$, dist[u][v] contains the shortest path $u \rightsquigarrow v$ consisting of intermediate vertices from 1 to $k+1$.

By induction on $k$, after iteration $n$, dist[u][v] contains the length of a shortest path $u \rightsquigarrow v$ consisting of any intermediate vertices, hence the distances are correct.

## Transitive closure

**Definition: Transitive Closure**

The transitive closure of a graph $G$ is a new graph $G'$ on the same vertices such that there is an edge $(u, v)$ in $G'$ if and only if there is a path between $u$ and $v$ in $G$.

Finding the transitive closure of a graph can be reduced to the problem of finding all-pairs shortest paths by noting that there is an edge between $u$ and $v$ in the transitive closure if and only if dist[u][v] $< \infty$. We can save some space by observing that we only ever care about whether or not two vertices are connected, not what their distance value is. Given this, we can store our connectivity matrix using single bits for each entry (a data structure called a *bitset* or *bitvector* in some languages,) where 0 means disconnected and 1 means connected, and update them by noting that vertex $u$ is connected to vertex $v$ via vertex $k$ if and only if connected[i][k] and connected[k][j] are both true. The space complexity of the algorithm therefore becomes $O\left(|V|^2/w\right)$, where $w$ is the number of bits in a machine word. The time complexity can also be improved to $O\left(|V|^2/w\right)$ by using integer bitwise operations, but we won't discuss that for now.

**Algorithm 64** Warshall's transitive closure algorithm

```
1:  function TRANSITIVE_CLOSURE(G = (V, E))
2:      Set connected[1..n][1..n] = False      // Store using a bitvector
3:      Set connected[v][v] = True for all vertices v
4:      Set connected[u][v] = True for all edges e = (u,v) in E
5:      for each vertex k = 1 to n do
6:          for each vertex u = 1 to n do
7:              for each vertex v = 1 to n do
8:                  connected[u][v] = connected[u][v] or (connected[u][k] and connected[k][v])
9:              end for
10:         end for
11:     end for
12:     return connected[1..n][1..n]
13: end function
```

# Chapter 14

# Dynamic Connectivity in Graphs

Connectivity in undirected graphs is a simple but widely applicable problem. We've seen how to find the connected components of a graph using depth-first search. Once the components have been identified, the problem of determining whether various pairs of nodes are connected can then be solved in constant time. The problem becomes much more difficult once we allow the graph to modified in between queries. This problem is called the dynamic connectivity problem, and we are going to see an optimal solution to the simplest variant of it; incremental connectivity. The incremental connectivity problem can be solved by reducing it to the disjoint set problem, which can be solved fast using a data structure called union-find.

**Summary: Dynamic Connectivity**

In this chapter, we cover:

- Connectivity in undirected graphs
- The dynamic connectivity problem
- The union-find linked list data structure
- The union-find forest data structure (**Not examinable in Semester Two, 2018**)

**Recommended Resources: Dynamic Connectivity**

- CLRS, Introduction to Algorithms, Chapter 21
- Weiss, Data Structures and Algorithm Analysis, Chapter 8
- `https://visualgo.net/en/ufds` - Visualisation of union-find

## Connectivity in Graphs

Two vertices $u, v$ in a graph $G$ are considered to be *connected* if there exists a path between them. This can be determined in linear time by running a search from $u$ or $v$ and checking whether the other vertex gets visited. Of course, if we wish to check large numbers of pairs of vertices, doing a search each and every time would be redundant and inefficient. A better solution is to first find the connected components of the graph, which can be done in linear time with a depth-first or breadth-first search. Recall Algorithm 53 from Chapter 12.

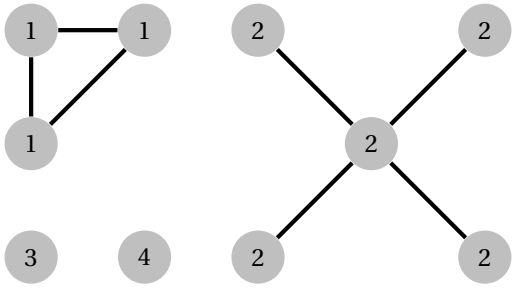



Figure 14.1: An undirected graph where each vertex is labelled by its connected component number. Note that two vertices are connected if and only if they have the same number.

With the connected components known, each connectivity query can be answered in constant time by simply checking whether the two vertices are assigned to the same component or not.

**Algorithm 65** Connectivity check

```
1: function CONNECTED(u, v)
2:     return (component[u] = component[v])
3: end function
```

The problem becomes much more interesting (and difficult) if we want to modify the graph in between queries. One solution is to simply recompute the connected components each time we make a modification, but this will get expensive if we begin to make lots of them. This problem is called the *dynamic connectivity* problem.

## The Dynamic Connectivity Problem

The dynamic connectivity problem is the problem of determining whether two vertices $u, v$ in a graph $G$ are connected, while allowing the graph $G$ to be modified, that is, have edges inserted and deleted in between queries. Simply rerunning the connected components algorithm every time we make a modification is inefficient, so we'd like to find a better way to approach the problem. The fully general dynamic connectivity problem is quite tricky, so we will focus our efforts on the simplest but arguably most useful variant of the problem, the *incremental connectivity* problem, in which we are only allowed to add edges, but not remove them.

### The incremental connectivity problem

The incremental connectivity problem is the problem of finding a data structure that can support the following two operations:

1. CONNECTED(u, v): Check whether the vertices u and v are connected.
2. LINK(u, v): Add an edge between the vertices u and v.

We'd like to perform these operations fast, so simply doing a search per CONNECTED query or recomputing every connected component per LINK query is too slow. This problem can be solved efficiently using a data structure called a *union-find* or *disjoin-set* data structure.

## The Union-Find Disjoint-Set Data Structure

The *union-find* or *disjoin-set* data structure is a data structure for maintaining a collection of $n$ elements, each of which belongs to a single set, that allows us to merge the contents of some pair of sets together. Each disjoint set is identified by a *representative*, which is some arbitrary but consistent element of that set.

Formally, the operations supported by a union-find structure are:

1. FIND(u): Determine which set a particular element is contained in. Usually this means finding the representative of the set.
2. UNION(u, v): Join the contents of the sets containing u and v into a single set.

These two operations can be seen as equivalent to maintaining the connected components of an undirected graph, where each item in a set represents a vertex, and each union operation represents the addition of an edge which might connect two components. Checking whether two vertices are in the same connected component then reduces to checking whether they have the same representative, i.e. whether FIND(u) = FIND(v).

### The first approach - disjoint set linked lists

One simple but suboptimal way to implement a union-find structure is to use linked lists. Each list represents one disjoint set, with each node of the list representing one of the items in the set. The head (first) element of the linked list is chosen to be the representative for each disjoint set.

1. FIND(u): To find the representative of $u$, we simply traverse to the head of the linked list containing $u$.
2. UNION(u, v): To merge the sets containing $u$ and $v$, we first check that they are not already contained in the same set, and if not, simply append the two linked lists containing them together.

In the worst case, both of these operations cost $O(n)$, which is no good. Several optimisations can be made to improve the performance of this implementation.

1. We can maintain for each element, a pointer to its representative, making us able to answer FIND queries in constant time
2. We can also track the length of each list, and make UNION faster by always choosing to append the smaller list to the larger one. This is called the weighted-union heuristic.

It can be shown that using these two heuristics results in a total complexity of $O(n \log(n))$ to perform union $n-1$ union operations in the worst case, which is $O(\log(n))$ on average per union. This is pretty good, but we can do even better.

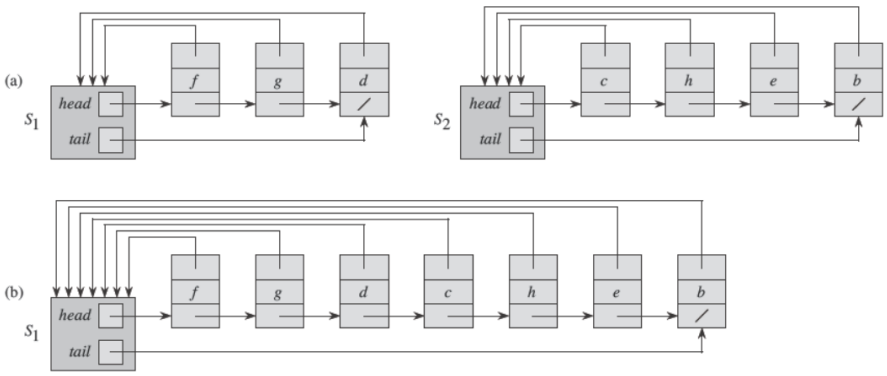



Figure 14.2: A linked list representation of a disjoint set data structure. The result of merging the two sets shown in (a) is depicted by (b). Figure source: CLRS

## A better approach - disjoint set forests (Not examinable in Semester Two, 2018)

Rather than represent each set by a linked list, a faster version of union-find represents each set by a rooted tree, where each node represents one element and the root node is taken to be the representative element. For each node in the forest, all that we need to store is a pointer to its parent in its tree. If a node is a root node, then we traditionally set its parent pointer to point to itself to indicate this. The disjoint set operations are then supported like this:

1. FIND(u): To find the representative of $u$, we simply follow the parent pointers until we reach the root of the tree containing it.
2. UNION(u,v): To merge the sets containing $u$ and $v$, we first check that they are not already contained in the same set, and if not, point the root node of one of the trees to the root node of the other, making one tree a subtree of the other.

An implementation is depicted in Algorithm 66. So far, this does not improve on the linked list implementation, since a sequence of union operations may result in a tree of breadth one, which is functionally identical to a linked list. Several optimisations can be made though which result in the forest implementation achieving significantly better performance than the linked list implementation.

### The path compression technique

The first and most important technique that we can apply to speed up union-find is *path compression*. The effect of path compression is very simple, whenever we perform the FIND operation to locate the root of a particular node's tree, we might as well point each node on the path directly at the root, so that whatever path we had to traverse will never have to be traversed again. This has the effect of flattening the tree and removing long chains, which significantly speeds up future FIND queries. It can be shown that with path compression, the worst-case cost of performing $m$ operations is $O(m\log(n))$, i.e. at most $O(\log(n))$ on average.

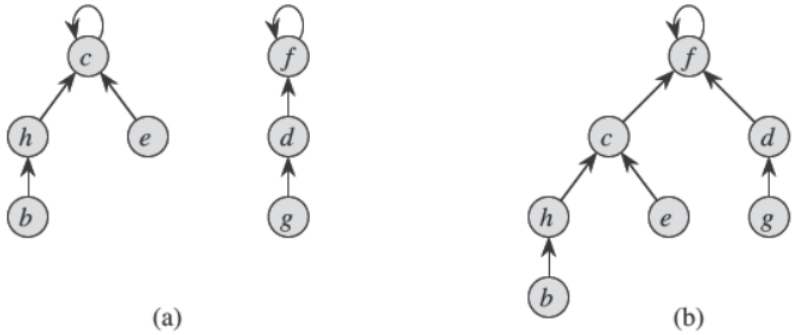



Figure 14.3: A forest representation of a disjoint set data structure. The result of merging the two sets shown in (a) is depicted by (b). The left tree has become a subtree of the right tree. Figure source: CLRS

**Algorithm 66** Union-find using disjoint-set forests (without optimisations)

```
1:  function INITIALISE(n)
2:      Set parent[1..n] = 1..n
3:  end function
4:
5:  function FIND(x)
6:      if parent[x] = x then return x
7:      else return FIND(parent[x])
8:  end function
9:
10: function UNION(x, y)
11:     parent[FIND(x)] = FIND(y)
12: end function
```

#### The union-by-rank technique

Union by rank is a similar heuristic to the weighted-union heuristic used in the linked list implementation. In union by rank, we maintain a "rank" for each tree, which is an upper bound on the height of the tree. When merging two trees together, we choose to always make the tree with a smaller rank a child of the tree with the larger rank. This ensures that the height of the resulting tree is no bigger than the constituent trees, unless they were of the same height. It can be shown that with union by rank, the worst-case cost of performing $m$ operations is also $O(m\log(n))$, i.e. at most $O(\log(n))$ on average.

#### Combining path compression union by rank

Combining the two heuristics together can be shown to yield even better performance. In the worst case, a sequence of $m$ operations will cost $O(m\alpha(n))$, or $\alpha(n)$ on average, where $\alpha(n)$ is

the inverse Ackermann function, an extremely slowly growing function. To put it in perspective, $\alpha(n) \leq 4$ for all values of $n$ that can be written in the universe (their number of digits is bounded by the number of atoms in the universe) so we can view it as constant for all practical (but not theoretical) purposes. This is a significant improvement over the $O(\log(n))$ complexity of disjoint set linked lists. This complexity bound also turns out to be provably optimal, in other words, no disjoint-set data structure can possibly do better than this.

**Algorithm 67** The FIND operation using path compression

```
1: function FIND(x)
2:     if parent[x] ≠ x then parent[x] = FIND(parent[x])
3:     return parent[x]
4: end function
```

**Algorithm 68** The UNION operation using union by rank

```
1: function INITIALISE(n)
2:     Set parent[1..n] = 1..n
3:     Set rank[1..n] = 0
4: end function
5:
6: function UNION(x, y)
7:     x = FIND(x)
8:     y = FIND(y)
9:     if rank[x] < rank[y] then
10:        parent[x] = y
11:    else
12:        parent[y] = x
13:        if rank[x] = rank[y] then
14:            rank[x] += 1
15:        end if
16:    end if
17: end function
```

# Chapter 15

# Minimum Spanning Trees

The minimum spanning tree problem is informally, the problem of finding the cheapest way to connect a set of nodes in a network. Minimum spanning trees arise in applications such as connecting cables in a network, where several locations need to be connected together at a minimum possible cost. We will see two algorithms for solving the minimum spanning tree problem, Prim's algorithm which is very similar to Dijkstra's, and Kruskal's algorithm which makes use of the union-find data structure.

**Summary: Minimum Spanning Trees**

In this chapter, we cover:

- The concept of a minimum spanning tree
- Prim's algorithm for minimum spanning trees
- Kruskal's algorithm for minimum spanning trees

**Recommended Resources: Minimum Spanning Trees**

- CLRS, Introduction to Algorithms, Chapter 23
- Weiss, Data Structures and Algorithm Analysis, Section 9.5
- `https://visualgo.net/en/mst` - Visualisation of minimum spanning trees
- `https://youtu.be/tKwnms5iRBU` - MIT 6.046 lecture on MSTs
- `http://users.monash.edu/~lloyd/tildeAlgDS/Graph/Undirected/`

## Minimum Spanning Trees

A spanning tree of a graph $G = (V, E)$ is a subgraph $T$ consisting of all of the same vertices $V$ and some subset $E' \subset E$ of the edges such that $T$ is a tree. Informally, it is a subset of the edges in $E$ that connect all of the vertices in $V$. Since spanning trees are trees, they are acyclic (they do not contain cycles.) A spanning tree of an edge-weighted graph is called a weighted spanning tree, and a weighted spanning tree with minimum possible total weight is called a minimum spanning tree. In other words, a minimum spanning tree is a connected subgraph

that minimises the total weight

$$w(T) = \sum_{(u,v) \in E(T)} w(u,v).$$

Although the definition of a minimum spanning tree is a global one, that is we are required to minimise the total weight of the tree, minimum spanning trees have local structure which allows us to find them using greedy algorithms. We will see two such greedy algorithms, Prim's algorithm which is almost identical to Dijkstra's algorithm, and Kruskal's algorithm which makes use of the union-find disjoint-set data structure. For both algorithms presented below, we assume that the graph $G$ is connected (otherwise no spanning trees exist).

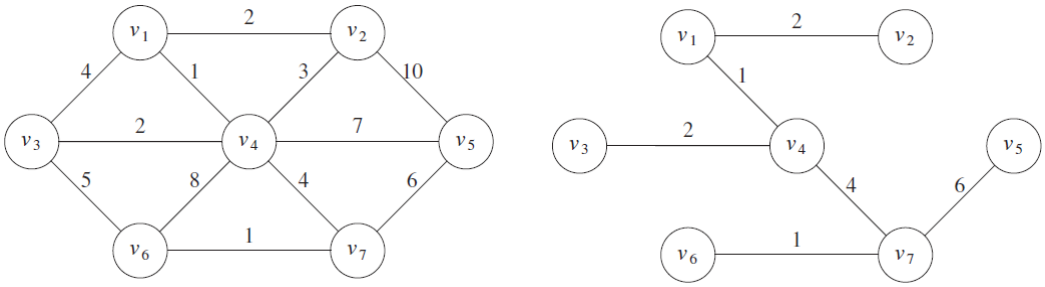



Figure 15.1: A weighted graph $G$ and a minimum spanning tree of $G$. Image source: Weiss

## Prim's Algorithm

Prim's algorithm for minimum spanning trees is very similar to Dijkstra's algorithm for single-source shortest paths. Prim's algorithms begins with an arbitrarily chosen source vertex and builds a tree $T$, adding edges one at a time to to form a spanning tree. The edge to add at each iteration is chosen such that it is a lightest weight edge that connects the current partial spanning tree $T$ to some new vertex $v$ not yet in the tree. To contrast, while Dijkstra's algorithm forms a shortest path tree by selecting a vertex with the smallest total distance from the source, Prim's selects a vertex with minimum possible distance to $T$. An implementation is given in Algorithm 69. Observe the similarity to Dijkstra's algorithm. Note that we may choose the root node $r$ to be any node in the graph.

### Complexity of Prim's algorithm

Compare the code for Prim's to that of Dijkstra's algorithm. The main difference is that the key used to greedily select the next vertex $v$ is taken to be the weight of the lightest edge $w(u,v)$ connecting $v$ to the current tree, rather than the total distance from $v$ to the source node. Otherwise, the two algorithms are almost identical. Like Dijkstra's algorithm, the complexity of Prim's algorithm using a binary heap to implement the priority queue is therefore $O(|E|\log(|V|))$.

**Algorithm 69** Prim's algorithm

```
1:  function PRIM(G = (V, E), r)
2:      Set dist[1..n] = ∞
3:      Set parent[1..n] = null
4:      Set T = ({r}, ∅)
5:      Set dist[r] = 0
6:      Set Q = priority_queue(V[1..n], key(v) = dist[v])
7:      while Q is not empty do
8:          u = Q.pop_min()
9:          T.add_vertex(u)
10:         T.add_edge(parent[u], u)
11:         for each edge e = (u,v) adjacent to u do
12:             if not v ∈ MST and dist[v] > w(u,v) then
13:                 // Remember to update the key of v in the priority queue
14:                 dist[v] = w(u,v)
15:                 parent[v] = u
16:             end if
17:         end for
18:     end while
19:     return T
20: end function
```

## Correctness of Prim's algorithm

We prove the correctness of Prim's algorithm by describing an invariant that it maintains.

**Theorem: Invariant of Prim's algorithm**

Every iteration of Prim's algorithm, the current set of selected edges $T$ is a subset of some minimum spanning tree of $G$.

**Proof**

Initially $T$ is empty, so $T$ is a subset of some MST of $G$. Suppose that at some iteration, $T$ is a subset of some MST. Denote this MST by $M$. Let $e = (u, v)$ denote the lightest edge that connects some $u \in T$ to some $v \notin T$. If $M$ contains $e$ then $T \cup \{e\}$ is a subset of some MST, so the invariant holds. Otherwise, suppose that $M$ does not contain $e$. We need to prove that there exists some other MST such that $T \cup \{e\}$ is a subset of it.

Since $M$ is a tree, it contains a path $p$ from $u \rightsquigarrow v$. Since $u$ and $v$ are not connected in $T$, at least one of the edges on the path $p$ is not contained in $T$. Let $(x, y)$ be the first edge on the path $p$ from $u$ to $v$ that is not contained in $T$. Since $(x, y)$ is the first edge not in $T$, and $T$ is a subset of $M$, $x \in T$ and $y \notin T$.

Since $M$ is a tree, removing the edge $(x, y)$ disconnects $M$ into two components $M_1$ and $M_2$. Connecting the edge $(u, v)$ to $M_1$ and $M_2$ reconnects them to form a new spanning

tree $M' = M_1 \cup M_2 \cup \{(u,v)\} = M \cup \{(u,v)\} \setminus \{(x,y)\}$. Since $(u,v)$ is the lightest edge connecting $T$ to a new vertex, it is no heavier than $(x,y)$, otherwise Prim's would have picked $(x,y)$ instead since $x \in T$ and $y \notin T$. In other words, $w(u,v) \leq w(x,y)$, which implies that $w(u,v) - w(x,y) \leq 0$. So the total weight of $M'$ is

$$\begin{aligned} w(M') &= w(M) + w(u,v) - w(x,y) \\ &\leq w(M) \end{aligned}$$

But since $M$ is a minimum spanning tree $w(M) \leq w(M')$ and hence $w(M) = w(M')$, from which we conclude that $M'$ is also a minimum spanning tree. Since $T \cup \{e\}$ is a subset of $M'$, we have shown that the invariant is maintained.

**Corollary: Correctness of Prim's algorithm**

Prim's algorithm correctly produces a minimum spanning tree.

**Proof**

First, we argue that Prim's algorithm produces a spanning tree. Whenever Prim's adds an edge to the MST, it does so to a newly added vertex, which means it can never create a cycle. Since the graph is connected, Prim's will visit every vertex and hence it will produce a spanning tree. Therefore when the algorithm terminates, $T$ is a spanning tree, and by the invariant above, it is a subset of some minimum spanning tree. Since all spanning trees contain the same number of edges, $T$ itself must be a minimum spanning tree. Hence Prim's algorithm is correct.

## Kruskal's Algorithm

Kruskal's algorithm like Prim's also greedily selects edges, but using a different strategy. Instead of building a single tree and growing it larger each iteration, Kruskal's algorithm instead maintains a forest $F$ of minimum weight subtrees. At each iteration, Kruskal's algorithm selects the lightest weight edge that connects two currently disconnected subtrees. In order words, Kruskal's selects the minimum weight edge that does not induce a cycle in the current forest. In order to quickly check whether or not an edge will connect two currently disconnected vertices, we utilise the union-find disjoint sets data structure. See the implementation in Algorithm 70.

### Complexity of Kruskal's algorithm

Sorting the edges of the graph takes $O(|E|\log(|E|))$ time, and the sequence of UNION and FIND operations takes $O(|E|\log(|V|))$. The total time complexity of Kruskal's algorithm is therefore $O(|E|\log(|E|))$, or equivalently $O(|E|\log(|V|))$ since $\log(E) = O(\log(|V|^2)) = O(|\log(|V|))$ in a simple graph.

**Algorithm 70** Kruskal's algorithm

```
1:  function KRUSKAL(G = (V, E))
2:      sort(E, key((u,v)) = w(u, v))        // Sort edges in ascending order of weight
3:      forest = UnionFind.initialise(n)
4:      Set T = (V, ∅)
5:      for each edge (u,v) in E do
6:          if forest.find(u) ≠ forest.find(v) then        // Ignore edges that would create a cycle
7:              forest.union(u, v)
8:              T.add_edge(u, v)
9:          end if
10:     end for
11:     return T
12: end function
```

## Correctness of Kruskal's algorithm

We prove the correctness of Kruskal's algorithm by using an invariant. In fact, it is the same invariant as maintained by Prim's, and the proof is almost identical.

**Theorem: Invariant of Kruskal's algorithm**

Every iteration of Kruskal's algorithm, the current set of selected edges $T$ is a subset of some minimum spanning tree of $G$.

**Proof**

Initially $T$ is empty, so $T$ is a subset of some MST of $G$. Suppose that at some iteration, $T$ is a subset of some MST. Denote this MST by $M$. Let $e = (u, v)$ denote the lightest edge that connects two vertices that are not yet connected in $T$. If $M$ contains $e$ then $T \cup \{e\}$ is a subset of some MST, so the invariant holds. Otherwise, suppose that $M$ does not contain $e$. We need to prove that there exists some other MST such that $T \cup \{e\}$ is a subset of it.

Since $M$ is a tree, it contains a path $p$ from $u \rightsquigarrow v$. Since $u$ and $v$ are not connected in $T$, at least one of the edges on the path $p$ is not contained in $T$. Let $(x, y)$ be any edge on the path from $u$ to $v$ that is not contained in $T$. Since $T$ is a subset of $M$, the vertices $x$ and $y$ can not be connected in $T$ or $M$ would contain a cycle.

Since $M$ is a tree, removing the edge $(x, y)$ disconnects $M$ into two components $M_1$ and $M_2$. Connecting the edge $(u, v)$ to $M_1$ and $M_2$ reconnects them to form a new spanning tree $M' = M_1 \cup M_2 \cup \{(u, v)\} = M \cup \{(u, v)\} \setminus \{(x, y)\}$. Since $(u, v)$ is the lightest edge connecting two disconnected vertices in $T$, it is no heavier than $(x, y)$, otherwise Kruskal's would have picked $(x, y)$ instead since $x$ and $y$ are not connected in $T$. In other words, $w(u, v) \leq w(x, y)$, which implies that $w(u, v) - w(x, y) \leq 0$. So the total weight of $M'$ is

$$\begin{aligned} w(M') &= w(M) + w(u, v) - w(x, y) \\ &\leq w(M) \end{aligned}$$

But since $M$ is a minimum spanning tree $w(M) \leq w(M')$ and hence $w(M) = w(M')$, from which we conclude that $M'$ is also a minimum spanning tree. Since $T \cup \{e\}$ is a subset of $M'$, we have shown that the invariant is maintained.

**Corollary: Correctness of Kruskal's algorithm**

Kruskal's algorithm correctly produces a minimum spanning tree.

**Proof**

First, we argue that Kruskal's algorithm produces a spanning tree. $T$ will never contain a cycle since the use of the union-find data structure explicitly prevents it. $T$ must also be connected since $G$ is connected, and if there were two components that were not connected in $T$, Kruskal's would select the edge connecting them. Therefore when the algorithm terminates, $T$ is a spanning tree, and by the invariant above, it is a subset of some minimum spanning tree. Since all spanning trees contain the same number of edges, $T$ itself must be a minimum spanning tree. Hence Kruskal's algorithm is correct.

# Chapter 16

# Directed Acyclic Graphs

A directed acyclic graph (DAG) is a directed graph that contains no cycles. DAGs are useful for modelling many real-world problems, like tasks with prerequisite dependencies. DAGS also often admit simple and fast solutions to problems that are very difficult to solve on general graphs. We'll focus on two important properties of DAGs, topological ordering and critical (longest) paths.

**Summary: Directed Acyclic Graphs**

In this chapter, we cover:

- Directed acyclic graphs (DAGs) and their properties
- The topological sorting problem
- The critical path problem
- The relationship between DAGs and dynamic programming (just for fun)

**Recommended Resources: Directed Acyclic Graphs**

- CLRS, Introduction to Algorithms, Sections 22.4 and 24.2
- Weiss, Data Structures and Algorithm Analysis, Sections 9.2 and 9.3.4
- `https://visualgo.net/en/dfsbfs` - Visualisation of graph traversal
- `https://visualgo.net/en/sssp` - Visualisation of shortest paths
- `https://youtu.be/AfSk24UTFS8` - MIT 6.006 lecture on DFS
- `http://users.monash.edu/~lloyd/tildeAlgDS/Graph/DAG/`

## Directed Acyclic Graphs

A directed acyclic graph (DAG) is a directed graph that contains no cycles. DAGs are useful in particular for representing tasks that have prerequisites. For example, the units in your degree and their prerequisites form a DAG, where each edge denotes a unit that has another as a requirement. In project management, the tasks in a project might form a DAG which indicates which tasks must be performed before others. The two most fundamental and interesting problems on DAGs are the topological sorting problem and the critical path problem.

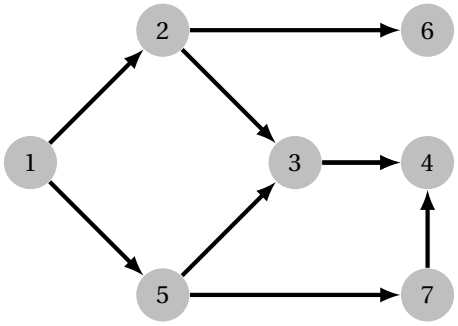
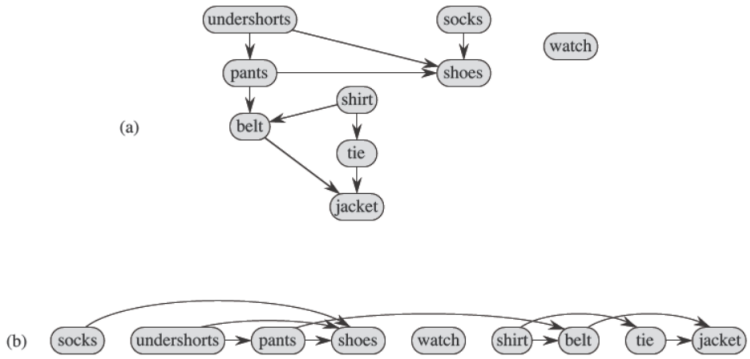



Figure 16.1: A directed acyclic graph.

# The Topological Sorting Problem

Given a DAG $G = (V, E)$, a topological ordering is a permutation of the vertices such that for any directed edge $e = (u, v)$, the vertex $u$ occurs before the vertex $v$. In other words, if the edges of the graph represent prerequisites, then a topological ordering represents a valid order in which to complete the tasks such that every prerequisite is satisfied. The topological sorting problem is the problem of producing a valid topological ordering for a given DAG.




A DAG (a) representing prerequisites for getting dressed and a correct topological ordering of the DAG (b). Image source: CLRS

## Kahn's algorithm for topological sorting

The most well-known algorithm for topological sorting is Kahn's algorithm, which maintains a queue of vertices that are ready to be completed and inserts them one by one into the topological ordering. A vertex is considered ready to be completed if it has no incoming edges (prerequisites) remaining. Once a vertex is taken and inserted into the ordering, any outgoing edges that it has are removed and its descendants are checked to see whether they are now ready too. An implementation is shown in Algorithm 71.

**Algorithm 71** Topological sorting using Kahn's algorithm

```
1:  function TOPOLOGICAL_SORT(G = (V, E))
2:      Set order = empty array
3:      Set ready = queue of all vertices with no incoming edges
4:      while ready is not empty do
5:          u = ready.pop()
6:          order.append(u)
7:          for each edge (u, v) adjacent to u do
8:              Remove (u, v) from G
9:              if v has no remaining incoming edges then
10:                 ready.push(v)
11:             end if
12:         end for
13:     end while
14:     return order
15: end function
```

Since Kahn's algorithm visits each vertex once and removes every edge once, its time complexity is $O(|V|+|E|)$ if implemented with the appropriate data structures. In practice, for efficiency, we do not actually delete edges from the graph during Kahn's algorithm. What we usually do is maintain an array that remembers the in-degree of every vertex (the number of incoming edges). Whenever we pop a vertex $u$, we decrease by one the in-degree of all vertices $v$ such that there exists an edge $(u, v)$. When this number hits zero, we know that the vertex is ready to be added to the queue.

### A depth-first search algorithm for topological sorting

Another useful algorithm for computing topological orderings is via a depth-first search. The key idea is that by performing a depth first search from some vertex $v$, we necessarily visit all of the vertices that depend on $v$. Therefore if during depth-first search we add each vertex to an array after we have finished visiting all of its descendants, its descendants will have already been added to the array before it, so the array will contain a reverse topological order. Since we are just performing a depth-first search and appending $|V|$ items to an array, the time complexity of this algorithm is also $O(|V|+|E|)$.

## The Critical Path Problem

The critical path problem is the problem of finding the **longest** path in a directed acyclic graph. This problem arises frequently in project management and operations research, where the vertices of a graph represent task completions and the edges represent tasks that must be completed, weighted by the amount of time that it will take to do so. The edges of the graph dictate the prerequisites of the tasks in the project. The longest path in the DAG therefore corresponds to the minimum amount of time in which the project can be completed if all prerequisites are obeyed.

**Algorithm 72** Topological sorting using DFS

```
1:  function TOPOLOGICAL_SORT(G = (V, E))
2:      Set order = empty array
3:      Set visited[1..n] = False
4:      for each vertex v = 1 to n do
5:          if not visited[v] then
6:              dfs(v)
7:          end if
8:      end for
9:      return reverse(order)
10: end function
11:
12: function DFS(u)
13:     visited[u] = True
14:     for each vertex v adjacent to u do
15:         if not visited[v] then
16:             dfs(v)
17:         end if
18:     end for
19:     order.append(v)        // Add to order after visiting descendants
20: end function
```

The critical path problem can be formulated as a simple dynamic programming problem. On a DAG, just like shortest paths, longest paths also admit substructure, i.e. any sub-path of a longest path must also be a longest path. Note that this is not true for a general graph (since general longest paths are not simple, i.e. they will contain duplicate edges unless the graph has no cycles), which is why longest path is not solvable in polynomial time in general.

For all vertices $u \in V$, let longest$[u]$ denote the length of the longest path that starts at $u$. Our base cases are all of the vertices with no outgoing edges, where longest$[v] = 0$. To determine the longest path that begins at some arbitrary vertex $u$, we simply consider all of the outgoing edges of $u$, and see which one yields the longest total path. In other words, we compute the dynamic program

$$\text{longest}[u] = \max_{v \in \text{adj}[u]} \big(w(u,v) + \text{longest}[v]\big).$$

The dependencies of the subproblems are clear from the graph, we must compute the longest path for all descendants of a node before we can compute the result for that node. In other words, the subproblems are dependant in a reverse topological order. Computing a topological order and iterating over every vertex and edge in the graph takes $O(|V|+|E|)$ time, hence we can solve the critical path problem in $O(|V|+|E|)$ time.

Since we are required to compute the topological order, we might as well solve the problem top-down recursively which removes the need to know the order of dependencies of the sub-problems. This results in a very short and elegant solution which also runs in $O(|V|+|E|)$ time.

**Algorithm 73** Bottom-up longest path in a DAG

```
1: function CRITICAL_PATH(G = (V, E))
2:     Set longest[1..n] = 0
3:     Set order = reverse(topological_sort(G))
4:     for each vertex u in order do
5:         for each edge (u, v) adjacent to u do
6:             longest[u] = max(longest[u], w(u, v) + longest[v])
7:         end for
8:     end for
9:     return longest[1..n]
10: end function
```

**Algorithm 74** Recursive longest path in a DAG

```
1: function CRITICAL_PATH(u)
2:     if longest[u] = null then        // longest[1..n] contains memoised subproblems
3:         Set longest[u] = 0
4:         for each edge (u, v) adjacent to u do
5:             longest[u] = max(longest[u], w(u, v) + CRITICAL_PATH(v))
6:         end for
7:     end if
8:     return longest[u]
9: end function
```

#### Relationship between topological orderings and dynamic programming

The recursive solution to the critical path problems reveals a very subtle but interesting fact about the relationship between depth-first search, topological orders, and dynamic programming. Take a look at the pseudocode in Algorithm 74. It looks a lot like the pseudocode for depth-first search (it is doing one after all), and it looks a lot like our top-down dynamic programming algorithms (which it is also).

Although it might not be immediately obvious, this problem actually illuminates a very interesting fact about dynamic programming that we saw when comparing top-down vs. bottom-up solutions. When computing a dynamic program bottom-up, it is necessary to know the order in which the subproblems are dependent on each other so that all of the necessary values are available when needed to compute each subsequent subproblem. When implementing a solution top-down however, we did not need to know the order of the subproblems since they would be computed precisely when needed.

The subproblems can not depend on each other cyclically, so their dependencies on each other actually form a DAG, where each subproblem is a vertex, and each dependency is a directed edge. The order in which we compute the subproblems must therefore be a valid topological order of that DAG. Whenever we compute a solution to a dynamic program using top-down recursion, we are actually performing a **depth-first search on the subproblem graph**, which means that we are actually producing a reverse topological order as a by-product! This explains why top-down solutions do not need to know a valid order in advance, because they are performing precisely the algorithm that computes one, even if we did not realise it.

This realisation allows us to rephrase many dynamic programming problems as path problems on DAGs. For example, recall the coin change problem from Chapter 5. If we construct a graph $G$ where each node corresponds to a dollar amount $\$V$, and add edges between the dollar amounts $(V, V-c_i)$ for all coin denominations $c_i$ and all dollar amounts $V$, then the coin change problem is precisely the problem of finding the shortest path from the desired dollar amount in this DAG to the \$0 vertex!

# Chapter 17

# Network Flow

Network flow models describe the flow of some material through a network with fixed capacities, with applications arising in several areas of combinatorial optimisation. On the surface, network flow can be used to model fluid in pipes, telecommunication networks, transport networks, financial networks and more. Beyond its obvious applications however, network flow turns out to be useful and applicable to solving a large range of other combinatorial problems, including graph matchings, scheduling, image segmentation, project management, and many more problems that do not initially sound like they have anything to do with flows.

**Summary: Network Flow**

In this chapter, we cover:

- Network flow and the maximum flow problem
- The Ford-Fulkerson algorithm for maximum flow
- The minimum cut problem
- The min-cut max-flow theorem
- The bipartite matching problem and its solution using max flow

**Recommended Resources: Network Flow**

- CLRS, Introduction to Algorithms, Chapter 26
- Weiss, Data Structures and Algorithm Analysis, Section 9.4
- `https://visualgo.net/en/maxflow` - Visualisation of maximum flow
- `https://visualgo.net/en/matching` - Visualisation of bipartite matching
- `https://youtu.be/VYZGlgzr_As` - MIT 6.046 lecture on maximum flow

## Network Flow Problems

Consider a road network consisting of towns connected by roads, along each of which a company can send up to a certain number of trucks per day. Our trucking company wants to know the maximum number of trucks that they can send per day from Vancouver to Winnipeg if they distribute them optimally. See the example in Figure 17.1.

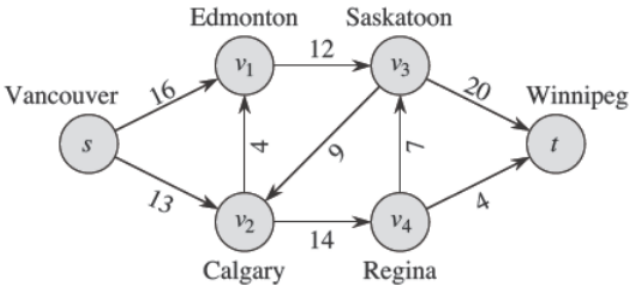



Figure 17.1: A road network of major cities in Canada. The edge weights represent the capacity of the roads, say the number of trucks that can be sent along that particular road per day. Image source: CLRS

In this case, an optimal solution turns out to be to send:

- 12 trucks from Vancouver to Edmonton,
- 12 trucks from Edmonton to Saskatoon,
- 19 trucks from Saskatoon to Winnipeg,
- 11 trucks from Vancouver to Calgary,
- 11 trucks from Calgary to Regina,
- 7 trucks from Regina to Saskatoon,
- 4 trucks from Regina to Winnipeg,

which results in a total flow of 23 trucks per day. See Figure 17.2.

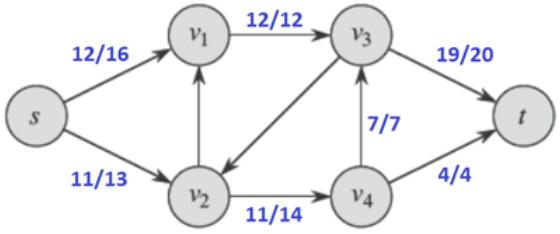



Figure 17.2: An optimal solution to the road network problem in Figure 17.1. A label of $x/y$ indicates that we send $x$ trucks along the road which has capacity $y$. Image source: Adapted from CLRS

A similar problem might be to consider a computer network, consisting of computers (nodes) that are connected via a wired network. Each pair of connected computers can send messages to each other up to some fixed capacity, called their bandwidth. Given the bandwidths of each connection, we might want to find the total bandwidth between two computers given that we can send data along multiple different paths at the same time. See Figure 17.3.

All of these are examples of **network flow** problems. In short, we have a network consisting of nodes, one of which is the "source," the location at which the flow is produced, and the "sink,"

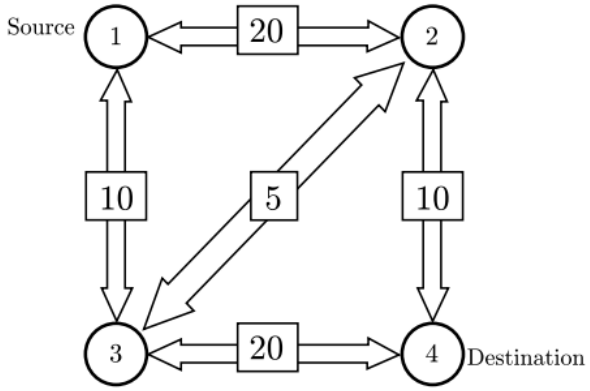



Figure 17.3: A computer network with edges labelled by the bandwidth of the connection between the two computers. The maximum possible bandwidth between the Source and the Destination is 25. Image source: ACM-ICPC World Finals 2000.

the location at which the flow is consumed. The problem that we will consider is the **maximum network flow** problem, or max-flow for short, where we are interesting in maximising the total amount of flow that can be sent from the source node to the sink node.

## Mathematical formulation as a linear program

The intuitive definition and examples above are more than enough to understand the maximum flow problem and the algorithms that we'll cover to solve it, but for completeness, here is the formal definition. It is not critical that you understand the formal definition, but it is very useful for proving things about the problem.

**Problem Statement: Maximum network flow problem**

Let $G = (V, E)$ be a directed, edge-weighted network with two special vertices $s$ and $t$, the source and sink respectively. Denote the capacity (edge weight) of an edge by $c(u, v)$. A flow $f$ in $G$ is a real-valued function

$$f : V \times V \to \mathbb{R}$$

that satisfies the following conditions:

- **Capacity constraint:** The flow along an edge must not exceed the capacity of that edge. Formally,
$$f(u, v) \leq c(u, v)$$
- **Flow conservation:** The amount of flow entering a node must be equal to the amount of flow leaving that node, with the exception of the source and sink. That

is for all $u \in V \setminus \{s,t\}$,

$$\sum_{v \in V} f(v,u) = \sum_{v \in V} f(u,v)$$

where $f(u,v) = 0$ if there is no edge $(u,v)$, i.e. if $(u,v) \notin E$.

The **value** of a flow $|f|$ is given by

$$|f| = \sum_{v \in V} f(s,v) - \sum_{v \in V} f(v,s)$$

The maximum flow problem then seeks to find a flow $f$ that maximises the value:

$$\max_{\text{flow} f} |f| \quad \text{subject to the } \textbf{capacity} \text{ and } \textbf{conservation} \text{ constraints.}$$

## The Ford-Fulkerson Algorithm

The Ford-Fulkerson algorithm, often referred to as the Ford-Fulkerson method since it encompasses a variety of potential implementations is one of the first and most intuitive algorithm for solving the maximum flow problem. Stated as briefly as possible, the algorithm is effectively:

*While more flow can be pushed through the network, push more flow through the network.*

Of course, we have to do some work to define what we really mean by pushing flow through a network, and to figure out how to find paths through which we are able to push flow. For example, simple naively pushing flow through the network until there is no longer a capacitated path from the source to the sink won't necessarily result in an optimal solution.

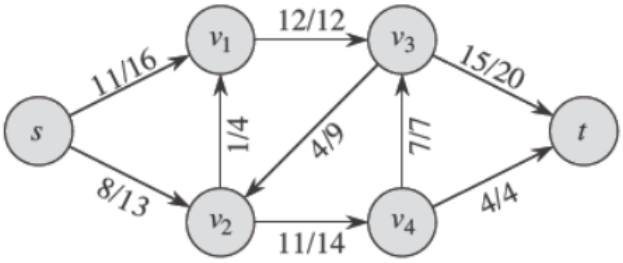



Figure 17.4: A flow on the road network from Figure 17.1. No more capacitated paths exist from the source to the sink, but the total flow of 19 is not optimal. In an optimal solution, we'd like to redirect the 4 flow that is going from $v_3$ to $v_2$ to go to $t$ instead. In other words, we need a way to send suboptimal flow choices back and redirect them. Image source: CLRS

To understand the Ford-Fulkerson method, we first need to define and explore the notion of the **residual network.**

## The residual network

Given a flow network $G = (V, E)$ and a flow $f$, the residual network $G_f$ essentially represents how much more flow can be sent through each edge. For example, an edge with capacity 9 and flow 4 has residual capacity 5, as 5 additional units of flow can be pushed along it. The residual capacity of an edge $(u, v)$ is given by

$$c_f(u, v) = c(u, v) - f(u, v).$$

Additionally, the residual network contains *back edges* or *reverse edges*, which are edges that flow in the opposite direction to those in $E$. The back edges are what allow the algorithm to "undo" flow by pushing flow back along the edge that it came from, and along a new direction instead. For each edge $(u, v)$ with positive flow $f(u, v)$, the residual network contains an edge $(v, u)$ with residual capacity

$$c_f(v, u) = f(u, v).$$

In other words, the back edge $(v, u)$ has the ability to cancel out the flow that currently exists on the edge $(u, v)$ by redirecting it down a different path.

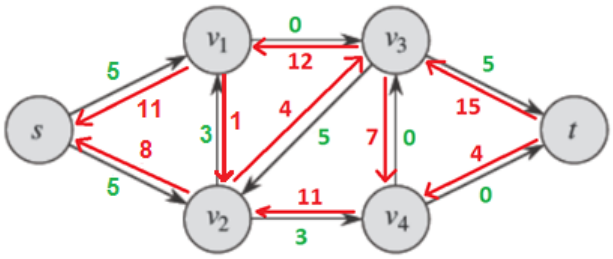



Figure 17.5: The residual network $G_f$ corresponding to the network and flow in Figure 17.4. The green labelled edges are the forward edges from $E$ with capacity $c(u, v) - f(u, v)$. The red edges are the back edges with capacity $f(v, u)$. Image source: Adapted from CLRS

## Augmenting paths

The example of the suboptimal flow in Figure 17.4 demonstrates that we can not always improve a flow by seeking a capacitated path in $G$. In order to increase the flow in a network, we instead seek *augmenting paths*, which are capacitated paths in the residual network $G_f$. An augmenting path may contain forward edges or back edges, which correspond to two situations:

- Augmenting along a forward edge simply corresponds to pushing more flow through that edge on the way from the source to the sink.
- Augmenting along a back edge corresponds to redirecting flow along that edge down a different path. The flow is reduced on the respective forward edge, and is moved to the remainder of the augmenting path.

Although the flow on the road network depicted in Figure 17.4 has no more capacitated paths from $s$ to $t$, the residual network does indeed have a capacitated path given by $s \to v_2 \to v_3 \to t$.

The total capacity of the path is the minimum capacity of the edges encountered along the path (that is the bottleneck of the path), as clearly we can send no more than this amount of additional flow along the path (or we would violate a capacity constraint.) Filling an edge to full capacity is often referred to as "saturating" the edge. Similarly, an edge is called saturated if the flow along it is at capacity.

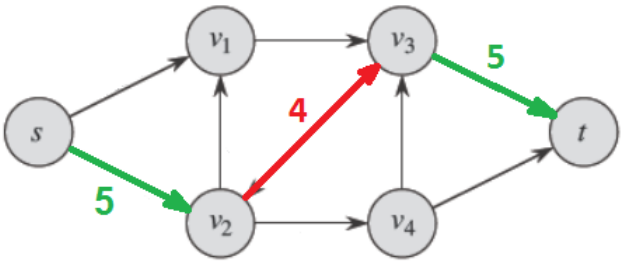



Figure 17.6: An augmenting path $p$ the in residual network $G_f$ in Figure 17.5. The total capacity of the augmenting path is 4, the bottleneck of the edge capacities in $p$. Image source: Adapted from CLRS

Augmenting 4 units of flow along the path $p$ depicted in Figure 17.6 will result in a total flow of 23 units which is now optimal. The key thing to understand here is that by augmenting along a back edge, we have redirected the flow that was once flowing along $v_3 \rightarrow v_2 \rightarrow v_4 \rightarrow t$ to flow directly from $v_3 \rightarrow t$ instead. As this flow is redirected away, the 4 units of flow that was being supplied to $v_2$ by $v_3$ is now supplied by $s$, so that the flow along $v_2 \rightarrow v_4 \rightarrow t$ is not reduced. Since any flow that is reduced by augmenting along a back edge always gets replaced, an augmentation always increases the total value of the flow.

## The method

We now have everything we need to describe the Ford-Fulkerson method. See the implementation in Algorithm 75. Of course, the Ford-Fulkerson method is really just a skeleton. The method tells us what to do, but does not specifically tell us **how** to do it. There are many possible strategies for actually finding augmenting paths, each of which will result in a different time complexity.

**Algorithm 75** The Ford-Fulkerson method

```
1: function MAX_FLOW(G = (V, E), s, t)
2:     Set initial flow f to 0
3:     while there exists an augmenting path p in the residual network G_f do
4:         Augment the flow f along the augmenting path p
5:     end while
6:     return f
7: end function
```

## Implementation using depth-first search

The simplest way to find augmenting paths in the residual network is to simply run a depth-first search on $G_f$. Before we present the implementation, lets just look at a few tricks that we use to make the algorithm easier to write.

**Use zero capacity edges to effectively represent back edges:** In a naive implementation, we might try to write separate code for dealing with forward edges and back edges, but we can actually use a very simple trick to make them work the same, eliminating repeated code. All we need to do is define the capacity of the back edges to be 0, and to maintain that their flow value is always equal to the negative of the flow on the corresponding forward edge. This works because the formula for residual capacity on an edge

$$c_f(u,v) = c(u,v) - f(u,v),$$

when applied to a back edge will yield

$$c_f(v,u) = c(v,u) - f(v,u) = 0 - (-f(u,v)) = f(u,v),$$

which is the definition of the residual capacity on a back edge. In other words, this formulation allows us to treat forward and back edges the same since the formula for their residual capacities is now the same.

**Augment flow in the same routine that finds an augmenting path:** Once an augmenting path has been found, we know that we are going to augment along it, so we might as well make our depth-first search that finds augmenting paths also perform the augmentation at the same time. Otherwise we would simply have to write twice the length of code where we would have to locate an augmenting path and then separately traverse it again to add flow.

**Edge structure:** Let's assume that we have an object structure representing an edge of the network, which contains the fields `capacity`, indicating the edge's capacity (remember that this will be zero for back edges), `flow`, which will indicate the current flow on that edge, and `reverse` which contains a reference to its reverse edge (the back-edge corresponding to the forward edge or vice versa).

Throwing all of these tricks together yields the pseudocode depicted in Algorithm 76

## Time Complexity

The time complexity of the Ford-Fulkerson algorithm depends on the strategy selected to find augmenting paths. Let's consider the simplest variant in which we use a depth-first search to find **any** augmenting path.

- Finding an augmenting path if one exists using a depth-first search from the source $s$ takes $O(|E|)$ time.
- In the worst case, each augmentation only increases the amount of flow by one unit[1], and hence it could take up to $|f|$ augmentations, where $|f|$ is the value of a maximum flow.

Therefore, the total time complexity of the Ford-Fulkerson algorithm is $O(|E| \times |f|)$.

[1] We have assumed for now that all capacities are integers. The maximum flow problem can in fact be generalised to consider non-integer capacities, although the Ford-Fulkerson algorithm is no longer guaranteed to work.

**Algorithm 76** Ford-Fulkerson implemented using depth-first search

```
1:  // DFS returns the capacity of the augmenting path found (or 0 if there are none left)
2:  function DFS(u, t, bottleneck)
3:      If u = t then return bottleneck        // We hit the sink, so we have an augmenting path
4:      visited[u] = True
5:      for each edge e = (u, v) adjacent to u do
6:          Set residual = e.capacity - e.flow
7:          if residual > 0 and not visited[v] then
8:              Set augment = DFS(v, t, min(bottleneck, residual))
9:              if augment > 0 then        // We found an augmenting path - add the flow
10:                 e.flow += augment
11:                 e.reverse.flow -= augment
12:                 return augment
13:             end if
14:         end if
15:     end for
16:     return 0        // We could not find an augmenting path
17: end function
18:
19: function MAX_FLOW(G = (V, E), s, t)
20:     Set flow = 0
21:     do
22:         Set visited[1..n] = False
23:         augment = DFS(s, t, ∞)
24:         flow += augment
25:     loop while augment > 0
26:     return flow
27: end function
```

## Better strategies for selecting augmenting paths

We can improve on the time complexity bound of $O(|E| \times |f|)$ by selecting better augmenting paths. We won't explore the details, but just summarise some of the common strategies:

- **Select shortest augmenting paths:** If we use a breadth-first search instead of a depth-first search, then we will find augmenting paths with the fewest number of edges. This is called the **Edmonds-Karp algorithm** and has a runtime complexity of $O(|V||E|^2)$.
- **Select augmenting paths with the largest capacity:** Finding a path with the maximum possible capacity can be achieved by finding a **maximum** spanning tree[2] in the residual graph $G_f$ with Prim's algorithm and then augmenting along the resulting path from $s$ to $t$. This is called the **fattest augmenting path algorithm** and results in a runtime of

$$O\left(|E|^2 \log(|V|) \log\left(|E| \max_{u,v \in V} c(u,v)\right)\right),$$

  which is better, although much trickier to read than the complexity of Edmonds-Karp!

[2] Exactly the same as a minimum spanning tree except selecting the heaviest edges instead of the lightest

## The Minimum Cut Problem

Given a flow network $G = (V, E)$ with edge capacities and a designated source vertex $s$ and sink vertex $t$, the minimum cut problem is the problem of finding a set of edges of minimum total capacity that if removed, would disconnect $s$ from $t$.

Let's illustrate this with a realistic example. Let's say you have a road network consisting of directed roads. Suppose that your tutor lives at vertex $s$ and that Monash University is at vertex $t$. You have a test coming up in your next lab, so you want to sabotage your tutor's chances of getting to the lab on time to avoid taking the test! For each directed road, you know the dollar amount that it would cost to have that road temporarily shut down and blocked off. What is the minimum amount of money that you'll have to spend in order to ensure that there is no way for your tutor to get to the university?

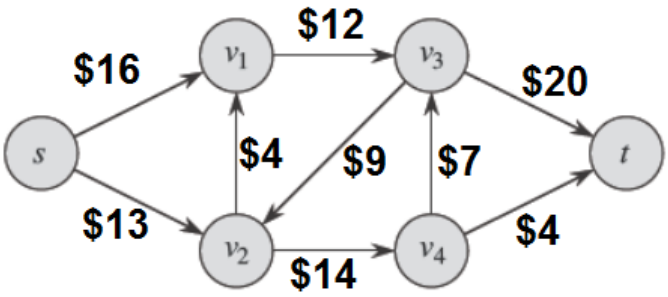



Figure 17.7: A road network, where edges are labelled by the cost of blocking off that particular road. Image source: Adapted from CLRS

This is precisely an example of a minimum cut problem. If we interpret the costs of blocking each road as the edges capacity, then the minimum cut is the cheapest way to disconnect $s$ from $t$. Consider the problem in Figure 17.7. By inspection, we can see that the minimum cut for the network above corresponds to blocking off the roads $v_1 \to v_3$, $v_4 \to v_3$ and $v_4 \to t$ for a total cost of $23.

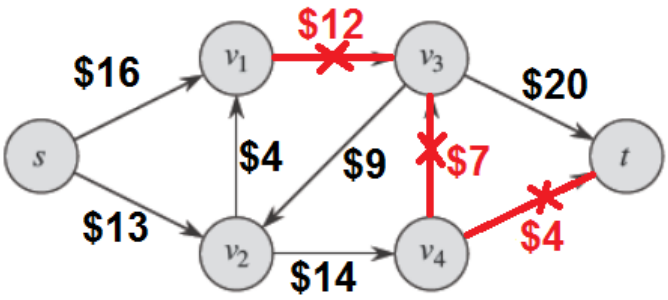



Figure 17.8: An optimal solution to the minimum cut problem. Image source: Adapted from CLRS

The minimum cut problem is intimately related to the maximum flow problem. Notice that

this road network is actually the same network that we used as an example for maximum flow in the previous section, whose maximum flow turned out to be exactly 23 units. This is not a coincidence.

## The min-cut max-flow theorem

One of the most interesting theorems in network theory is the **min-cut max-flow theorem.** Stated formally, the minimum cut problem is as follows.

**Problem Statement: Minimum cut problem**

Let $G = (V, E)$ be a directed, edge-weighted network with two special vertices $s$ and $t$, the source and sink respectively. Denote the capacity (edge weight) of an edge by $c(u, v)$.

An **s-t cut** $C = (S, T)$ is a partition of the vertices $V$ into two disjoint subsets $S$ and $T$ such that $s \in S$ and $t \in T$. The **capacity** of the cut $C$ is defined to be the total capacity of all edges that begin in $S$ and end in $T$, in other words, all edges that **cross** the cut. Formally,

$$c(S, T) = \sum_{u \in S} \sum_{v \in T} c(u, v)$$

where as usual, we take $c(u, v) = 0$ if there does not exist an edge $(u, v)$. The **minimum cut** problem seeks an s-t cut $C = (S, T)$ such that $c(S, T)$ is as small as possible.

The minimum cut problem and the maximum flow problem are related by the min-cut max-flow theorem. Informally, in a given flow network, the minimum cut and maximum flow problems have the same solution.

**Theorem: Min-cut max-flow theorem**

Given a flow network $G = (V, E)$ with a source vertex $s$ and sink vertex $t$, the value of a maximum s-t flow in $G$ is equal to the minimum capacity s-t cut in $G$. Mathematically:

$$\max_f |f| = \min_{(S,T)} c(S, T)$$

**Proof**

For a rigorous mathematical proof of the theorem, see CLRS, Theorem 26.6. We will consider a more intuitive version of the proof, which follows roughly the same structure as the formal proof, but using intuitive arguments in place of rigorous mathematical arguments.

If we consider a flow network $G$, some flow $f$ and some cut $(S, T)$, the net amount of flow that crosses the cut, i.e. moves through an edge from $S$ into $T$ must be equal to the value of the flow $|f|$. This has to be true because if $|f|$ total units of flow are moving from $s$ (contained in $S$) to $t$ (contained in $T$), then they must cross through the cut $(S, T)$. Given this, the value of the maximum flow can not be greater than the capacity of any

$(S, T)$ cut, since it must travel through it, so in particular, the value of the maximum flow must be less than or equal to the capacity of the minimum cut.

Consider a maximum flow $f$ and the particular s-t cut $(S, T)$ such that $S$ contains all vertices reachable from $s$ in the residual graph $G_f$, and $T$ contains all remaining vertices. $(S, T)$ is a valid cut since $t$ is not reachable from $s$, otherwise there would be an augmenting path, which would imply that the flow $f$ was not in fact maximum. Suppose that the value of $f$ was less than the capacity of $(S, T)$, i.e. that $|f| < c(S, T)$, then either there is an edge crossing $(S, T)$ that is not saturated, or there is an edge bringing flow from $T$ into $S$. If there is an unsaturated edge $(u, v)$ such that $u \in S$ and $v \in T$, then there is a path from $S$ to $T$ in the residual graph, which is a contradiction. Similarly, if there is an edge bringing flow from $T$ into $S$, then the corresponding back-edge from $S$ into $T$ has non-zero residual capacity, and hence there is a path from $S$ to $T$ in the residual graph, which is also a contradiction. Therefore, the value of the flow $f$ must be equal to the capacity of the cut $(S, T)$.

Since the value of the maximum flow $f$ can not exceed the capacity of any cut, and we have found a cut such that $|f| = c(S, T)$, we can conclude that the value of the maximum flow is equal to the capacity of the minimum cut.

Not only does the proof above illuminate why the theorem is true, it also shows us how to construct a minimum cut if we have found a maximum flow. If $G = (V, E)$ is a network and $f$ is the maximum flow, then the minimum cut $(S, T)$ can be found by taking $S$ equal to all of the vertices that are reachable from $s$ via the residual graph $G_f$, and taking $T$ as all remaining vertices. The proof shows that this will indeed be a minimum s-t cut in $G$. The min-cut max-flow theorem also gives us an easy tool to prove that the Ford-Fulkerson algorithm is correct.

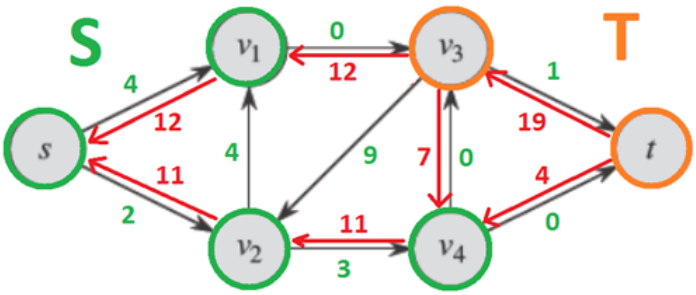



Figure 17.9: The residual network $G_f$ for the maximum flow in the network in Figure 17.7. The vertices reachable from $s$ are $\{s, v_1, v_2, v_4\}$, leaving $T = \{v_3, t\}$, across which, the capacity can be seen to equal to $12 + 7 + 4 = 23$, which agrees with the value of the maximum flow $f$. Image source: Adapted from CLRS

**Corollary: Correctness of Ford-Fulkerson**

Ford-Fulkerson terminates when there are no augmenting paths left. Since each augmenting path increases the flow by an integer, and the maximum flow is finite, the algorithm eventually terminates. When there does not exist an augmenting path from $s$ to $t$, the flow across the cut ($S = \{v : v$ reachable from $s$ in $G_f\}$, $T = V \setminus S$) is equal to the capacity of the cut. By the min-cut max-flow theorem, this flow is therefore maximum.

## Bipartite Matching

Recall that a bipartite graph is one where the vertices can be separated into two disjoint subsets $L$ and $R$ such that every edge connects a vertex $u \in L$ to a vertex $v \in R$.

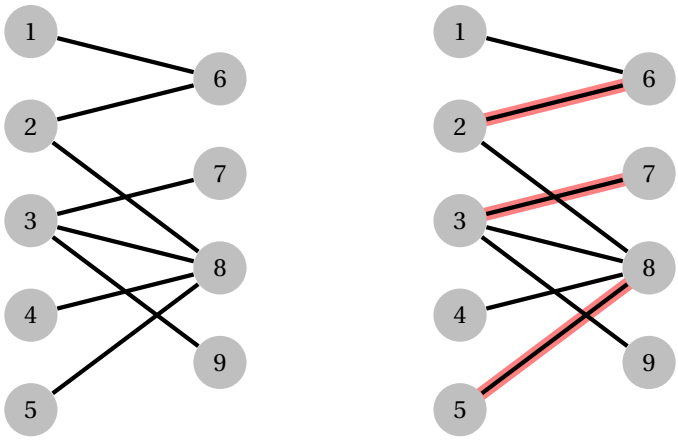



Figure 17.10: A bipartite graph composed of the two sides, $L = \{1,2,3,4,5\}$ and $R = \{6,7,8,9\}$, and a maximum matching which has size three.

Consider the example in Figure 17.10. Suppose that the set $L$ represents job applicants, and the set $R$ are available jobs. There is an edge between the applicant $u$ and the job $v$ if person $u$ is qualified for job $v$. The bipartite matching problem asks us to match qualified applicants to jobs such that no applicant gets multiple jobs, and no job is taken by multiple people. For this example, the greatest number of applicants that can be successfully matched is three.

**Problem Statement: Maximum bipartite matching**

Given a bipartite graph $B = (V, E)$, a **matching** is a subset $M$ of the edges $E$ such that no vertex $v \in V$ is incident to multiple edges in $M$. The maximum bipartite matching problem seeks a matching of the graph with the largest possible number of edges.

Although the maximum bipartite matching problem does not sound very similar to the maximum flow problem, it can actually be solved by constructing a corresponding flow network and

finding a maximum flow. The key idea is to use units of flow to represent matches. We construct the corresponding flow network by taking the bipartite graph $B = (V, E)$ and adding new sink ($s$) and source ($t$) vertices. We then connect the source vertex $s$ to every vertex in the left subset $L$ and connect every vertex in the right subset $R$ to the sink vertex $t$, and direct all of the original edges in $E$ to point from $L$ to $R$. We then finally assign every edge a capacity of one.

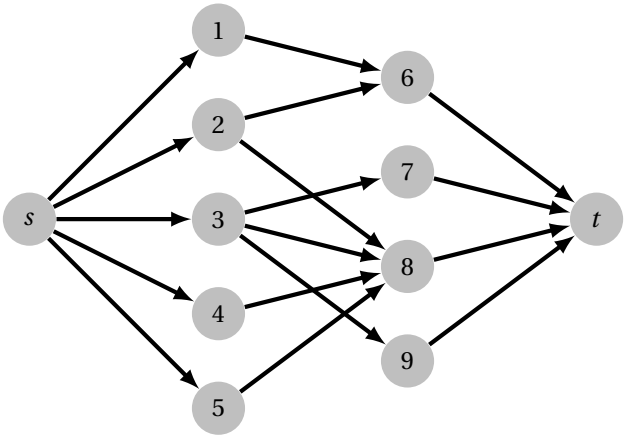



Figure 17.11: The corresponding flow network for the bipartite graph in Figure 17.10. Capacities are omitted since all edges have capacity 1.

Since every edge has a capacity of one, at most one unit of flow can be sent from $s$ through any vertex $u \in L$. This ensures that each applicant can get at most one job. Also,at most one unit of flow can leave any $v \in R$ into $t$, which ensures that each job gets at most one applicant. After finding a maximum flow, matches will correspond to edges from $L$ to $R$ that are saturated. The flow being a maximum flow ensures that the maximum possible number of matches are obtained.

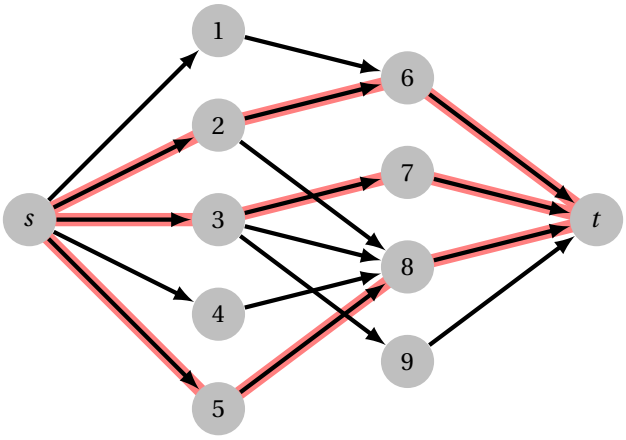



Figure 17.12: A maximum flow in the corresponding flow network. The highlighted edge are saturated with a flow of one, and form a maximum matching with size 3.

Given a bipartite graph $B = (V, E)$, the maximum possible number of matches can not be greater than the number of vertices, so the value of the flow in the corresponding flow network is bounded above by $|f| \leq |V|$. Using the Ford-Fulkerson algorithm to find the maximum flow therefore results in a runtime of $O(|V||E|)$ to solve the maximum bipartite matching problem. A faster algorithm called Hopcroft-Karp solves the maximum bipartite matching problem in $O(\sqrt{|V|}|E|)$ by using the same flow network but a faster maximum flow algorithm.

Using Ford-Fulkerson to find maximum matchings is sometimes called the *alternating paths algorithm* for bipartite matching, since the augmenting paths that will be found by Ford-Fulkerson will strictly alternate between the left and right parts of the graph using forward edges and back edges sequentially. In practical implementations of the algorithm, constructing the flow network explicitly is not required, and much unnecessary code can be avoided by simply keeping track of the matches such that augmenting paths can be found by beginning at an arbitrary unmatched vertex and traversing the graph, alternating between unmatched vertices on the left and matched vertices on the right until an unmatched vertex is discovered on the right.