Notes for Algorithms: Design and Analysis

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Chapter 1

Introduction

1.1 Warmup: Integer Multiplication Problem

1.1.1 The Primary School Approach

Consider the integer multiplication algorithm that everyone learned in primary school.

Input two n-digit numbers x and y.

Output the product $x \times y$.

We will assess its performance by counting the number of **primitive operations**, here being the addition or multiplication of two single-digit numbers, required to carry it out. In this case, it is clearly $\Theta(n^2)$. It might have been taken for granted that this is the unique, or at least optimal approach, while actually it isn't. As Aho, Hopcroft and Ullman put it in their 1974 book *The Design and Analysis of Computer Algorithms*, "Perhaps the most important principle for the good algorithm designer is to refuse to be content." Always be ready to ask yourself the question: CAN WE DO BETTER?

1.1.2 Karatsuba Multiplication

Consider the calculation of 5678×1234 . We will note a = 56, b = 78, c = 12 and d = 34. The calculation can be carried out with the following steps:

- 1. Calculate $a \cdot c = 672$;
- 2. Calculate $b \cdot d = 2652$;
- 3. Calculate $(a+b)(c+d) = 134 \times 46 = 6164$;
- 5. Calculate ①×10000 + ④×100 + ② = 6720000 + 284000 + 2652 = 7006652.

The procedure here can be formalized into a recursive algorithm to calculate $x \times y$. Write $x = 10^{n/2}a + b$ and $y = 10^{n/2}c + d$. Obviously we have $xy = 10^nac + 10^{n/2}(ad + bc) + bd = 10^nac + 10^{n/2}((a+b)(c+d) - ac - bd) + bd$, which inspires us of the following algorithm:

Algorithm 1.1 Karatsuba Multiplication

- 1: Recursively calculate *ac*;
- 2: Recursively calculate bc
- 3: Recursively calculate (a+b)(c+d)
- 4: Calculate ③ ② ① to get ad + bc
- 5: Combine the results appropriately, i.e. $xy = 10^n ac + 10^{n/2} (ad + bc) + bd$

Algorithm 1.1 demonstrates that even a simple problem with a presumably unique solution has plenty of room for subtle algorithm analysis and design.

1.2 Course Topic

The course will cover the following topics:

- Vocabulary for design and analysis of algorithms;
- Divide-and-conquer algorithm design paradigm;
- Randomization in algorithm design;
- Primitives for reasoning about graphs;
- Use and implementation of data structures.

In part II of the course the following topics will be covered:

- Greedy algorithm design paradigm;
- Dynamic programming algorithm design paradigm;
- NP-complete problems and what to do with them;
- Fast heuristics with provable guarantees for NP problems;
- Fast exact algorithms for special cases of NP problems;
- Exact algorithms that beat brute-force search for NP problems.

1.3 Merge Sort

We will use **merge sort** to illustrate a few basic ideas of the course. Merge sort is a non-trivial algorithm to tackle the sorting problem:

Input An unsorted array of n numbers;

Output The same numbers in sorted order.

1.3.1 Pseudo Code

Merge sort is more efficient than selection sort, insertion sort and bubble sort. It is a good introductory example for the divide & conquer paradigm. Its pseudo code is shown in Algorithm 1.2. The merging process may not seem intuitive.

```
Algorithm 1.2 Merge sort

input:

Unsorted array of length n

output:

Sorted array of length n

if length of the array = 0 or 1 then

return

Basic case. Array already sorted.

Recursively merge sort 1st half of the array.

Recursively merge sort 2nd half of the array.

Merge the two sorted halves into one sorted array.
```

It is implemented with parallel traverses of the two sorted sub-arrays, as shown in Algorithm 1.3.

```
Algorithm 1.3 Merging two sorted sub-arrays
```

```
input:
    A = 1st sorted sub-array, of length \lfloor n/2 \rfloor
    B = 2nd sorted sub-array, of length \lceil n/2 \rceil
output:
    C = sorted array of length n
 1: i = 1, j = 1
 2: for k = 1 to n do
 3:
        if i > A.len then
                                                             ▶ A has been exhausted
           C[k] = B[j++]
 4:
        else if j > B.len then
                                                             ▷ B has been exhausted
 5:
           C[k] = A[i++]
 6:
 7:
        else if A[i] < B[j] then
           C[k] = A[i++]
 8:
                                                                            \triangleright A[i] \ge B[j]
 9:
        else
           C[k] = B[j++]
10:
```

1.3.2 Running Time

The running time of the merging operation is obviously linear to the length of the array. Precisely speaking, each iteration involves one increment of i or j, one increment of k, an assignment to C[k] and at most 3 comparisons¹. Taking

¹Here we are taking an approach more detailed than that in the lecture: end cases, i.e. when A or B is exhausted, are taken into account.

the initialization of i and j into account, in total we have to carry out 6n + 2 primitive operations, which is smaller than 8n.

We can then draw the **recursive tree** of the problem. The original merge sort problem of size n resides at level 0. At level 1 we have 2 sub-problems of size n/2, etc. In general, at level j we have 2^j sub-problems of size $\frac{n}{2^j}$, and in total we have $\log n + 1$ levels². At each level, the number of required primitive operations is smaller than $8 \cdot \frac{n}{2^j} \cdot 2^j = 8n$. In the end, we have an upper bound of the total number of primitive operations needed to solve the original merge sort problem of size n: $8n(\log n + 1)$.

1.4 Asymptotic Analysis

In the analysis above, we have been applying 3 guiding principles that will serve as universal tactics in future analysis of algorithms:

- 1. Focus on worst-case analysis, rather than average-case analysis or benchmarks on a specified set of inputs.
- 2. Analyze with no regard to the constant factor.
- 3. Conduct asymptotic analysis, i.e. focus on running time when n is large.

Asymptotic analysis provides basic vocabulary for the design and analysis of algorithms. It is essential for high-level reasoning about algorithms because it is both coarse enough to suppress details dependent upon architecture, language, compiler and implementation details, and sharp enough to facilitate comparisons between different algorithms, especially for inputs of large size. Its high-level idea is to **suppress constant factors as well as lower-order terms**. For our example of merge sort, the running time of $8n(\log n + 1)$ is actually equivalent to $n \log n$, or in big-O notation, $O(n \log n)$.

1.4.1 Big-O Notation

Let $T(n), n \in \mathbb{N}$ be the function representing the running time of an algorithm with input of size n. The **Big-O notation** T(n) = O(f(n)) means that eventually (for all sufficiently large n), T(n) will be bounded above by a constant multiple of f(n). We hereby provide its formal definition.

Definition 1. Big-O notation T(n) = O(f(n)) holds if and only if there exist constants c, n_0 such that

$$T(n) \le c \cdot f(n), \forall n \ge n_0.$$

Theorem 1.

$$a_k n^k + \dots + a_1 n + a_0 = O(n^k)$$

²At the last level k we must have $\frac{n}{2^k} = 1$, thus $k = \log n$.

Proof. Constants
$$n_0 = 1$$
 and $c = \sum_{i=0}^{k} |a_i|$ satisfy Definition 1.

Theorem 2. For every $k \ge 1$, $n^k \ne O(n^{k-1})$.

Proof. The theorem can be proved by contradiction. Suppose $n^k = O(n^{k-1})$, i.e. \exists constants c, n_0 such that

$$n^k < c \cdot n^{k-1}, \forall n > n_0.$$

Then

$$n \leq c, \forall n > n_0,$$

which is an obvious contradiction.

1.4.2 Omega, Theta and Little-O Notations

Definition 2. Omega notation $T(n) = \Omega(f(n))$ holds if and only if there exist constants c, n_0 such that

$$T(n) \ge c \cdot f(n), n \ge n_0.$$

Definition 3. Theta notation $T(n) = \Theta(f(n))$ holds if and only if $T(n) = \Omega(f(n))$ and T(n) = O(f(n)), which is equivalent to \exists constants c_1, c_2, n_0 such that

$$c_1 \cdot f(n) \le T(n) \le c_2 \cdot f(n), \forall n \ge n_0$$

A convention in algorithm design, though a sloppy one, is to use big-O notation to represent Theta notation.

Definition 4. Little-O notation T(n) = o(f(n)) holds if and only if \forall constant c > 0, \exists constant n_0 such that

$$T(n) < c \cdot f(n), \forall n > n_0.$$

Theorem 3. $n^{k-1} = o(n^k), \forall k > 1$

Proof. Constant n=1/c can satisfy the condition.

Chapter 2

Divide and Conquer Algorithms

A typical divide-and-conquer solution to a problem consists of the following steps:

- 1. Divide the problem into smaller sub-problems.
- 2. Conquer the sub-problems via recursive calls.
- 3. Combine solutions of sub-problems into a solution to the original problem, often involving some clean-up work.

2.1 Inversion Counting Problem

We will solve the inversion problem using the divide-and-conquer paradigm. The problem is described as follow.

Input An array A containing numbers $1, 2, \ldots, n$ in some arbitrary order.

Output Number of inversions in this array, i.e. number of pairs [i, j] such that i < j and A[i] > A[j].

A geometrical solution to the problem is to draw two parallel series of points, mark one series in the order inside array A, and mark the other in the order $1, 2, \ldots, n$. Connect points marked by the same number, i.e. 1 with 1, 2 with 2, etc, then the number of crossing lines is exactly the number of inversions.

The inversion number is widely useful in comparison and recommendation systems. A movie rating website wants to compare tastes of its users and recommend to a user movies liked by other users with similar taste to his. One criterion of such comparison is to pick the ratings given by one user to a series of movies and compare them against other users' ratings by calculating the number of inversions. The fewer inversions there are, the more similar their tastes are.

A brute-force approach is obviously $\Theta(n^2)$. We can do better by applying the divide-and-conquer paradigm. Suppose that the array has been divided into two halves. An inversion [i,j] is called a left inversion if both i,j are in the left half, a right inversion if they are both in the right half, and a split inversion if i is in the left half and j is in the right half. A high-level divide-and-conquer algorithm is provided in Algorithm 2.1. If countSplitInv can be implemented as $\Theta(n)$, then the whole algorithm will be $\Theta(n \log n)$.

Algorithm 2.1 Divide-and-conquer Inversion Counting

```
input:
    Array A
output:
    Number of inversions in A
 1: function COUNT(Array A)
       if A.len == 1 then
 2:
 3:
          return 0
       else
 4:
          x = count(1st half of A)
                                                              ▶ Left inversions.
 5:
          y = count(2nd half of A)
                                                             ▶ Right inversions.
 6:
          z = countSplitInv(A)
                                                       ▷ Count split inversions.
 7:
 8:
          return x+y+z
```

The implementation of countSplitInv seems quite subtle, but it can actually be developed from merge sort. In Algorithm 2.1, the subroutine count only counts the number of inversions. In addition to that, we rename it with sortAndCount and require that it also sorts the array. Subroutine countSplitInv now becomes mergeAndCountSplitInv. It merges the two sorted sub-arrays into one sorted array and counts the number of split inversions.

If there exists no split inversion, it must be the case that any element of the left sub-array A is smaller than any element of the right sub-array B. As a result, when merging the two sorted sub-arrays, A will be exhausted before any element of B is put in the result. Once an element of B is chosen during the merging process before A is exhausted, every element left in A forms an inversion with it. Algorithm 2.2, developed from Algorithm 1.3, uses this idea to carry out the mergeAndCountSplitInv process. It is still $\Theta(n)$, thus our inversion counting algorithm is guaranteed to be $\Theta(n \log n)$.

2.2 Matrix Multiplication

Matrix multiplication is an important mathematical problem.

```
Input Two matrices X, Y of dimension N \times N.
```

Output Product matrix $Z = X \cdot Y$.

Algorithm 2.2 Merge and Count Split Inversion

```
input:
    A = 1st sorted sub-array, of length \lfloor n/2 \rfloor
    B = 2nd sorted sub-array, of length \lceil n/2 \rceil
output:
    C = sorted array of length n
    numSplitInv = number of split inversions
 1: i = 1, j = 1, numSplitInv = 0
 2: for k = 1 to n do
        if i > A.len then
 3:
                                                             ▶ A has been exhausted
           C[k] = B[i++]
 4:
        else if j > B.len then
                                                             ▷ B has been exhausted
 5:
           C[k] = A[i++]
 6:
        else if A[i] \leq B[j] then \triangleright In this case equality is actually impossible.
 7:
           C[k] = A[i++]
 8:
                                                                           \triangleright A[i] > B[j]
 9:
            C[k] = B[j++]
10:
           numSplitInv += A.len
11:
```

The definition of matrix multiplication is $Z_{ij} = \sum_{k=1}^{N} X_{ik} Y_{kj}$. Calculating the product matrix directly will result in a $\Theta(n^3)$ algorithm.¹ We will introduce an ingenious divide-and-conquer algorithm developed by Strassen that is more efficient.

At first sight, it might seem plausible to divide each matrix into 4 submatrices of dimension $N/2 \times N/2$ in the divide phase of the divide-and conquer process:

$$XY = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} E & F \\ G & H \end{pmatrix} = \begin{pmatrix} AE + BG & AF + BH \\ CE + DG & CF + DH \end{pmatrix}.$$

However, this division does not make great difference. The algorithm is still $\Theta(n^3)$, as we will prove later. Recall that in the Karatsuba Multiplication algorithm, we reduced the number of products by 1 by applying the Gauss's trick: obtain some products by linear combination of other products, rather than direct multiplication. Since addition/subtraction is generally more efficient than multiplication, it usually pays off to appropriately choose the products to calculate in order to reduce the number of products to calculate. In the naive divide-and-conquer design above, we have to calculate 8 products of submatrices. Strassen's brilliant algorithm reduces this number to 7, as shown in Algorithm 2.3, and ends up with smaller time consumption. The explanation of its time complexity, as well as that of the naive divide-and-conquer algorithm will be addressed later.

¹Here the input size is $\Theta(n^2)$, rather than $\Theta(n)$.

Algorithm 2.3 Strassen's Matrix Multiplication

input:

Two matrices X, Y of dimension $N \times N$ output:

Matrix product $X \cdot Y$

- 1: Divide the matrices: $X=\begin{pmatrix}A&B\\C&D\end{pmatrix},\,Y=\begin{pmatrix}E&F\\G&H\end{pmatrix}$
- 2: Recursively calculate

$$P_1 = A(F - H), P_2 = (A + B)H, P_3 = (C + D)E, P_4 = D(G - E)$$

 $P_5 = (A + D)(E + H), P_6 = (B - D)(G + H), P_7 = (A - C)(E + F)$

3: Linearly combine the products in step 2 to obtain XY:

$$XY = \begin{pmatrix} P_5 + P_4 - P_2 + P_6 & P_1 + P_2 \\ P_3 + P_4 & P_1 + P_5 - P_3 - P_7 \end{pmatrix} = \begin{pmatrix} AE + BG & AF + BH \\ CE + DG & CF + DH \end{pmatrix}$$

2.3 Closest Pair

The closest pair problem is the first computational geometry problem we meet.

Input A set of n points $P = \{p_1, \dots, p_n\}$ on the \mathbb{R}^2 plane. For simplicity, we assume that they have distinct x coordinates and y coordinates.

Output A pair of distinct points $p^*, q^* \in P$ that minimizes the Euclidean distance between two points d(p,q) with $p,q \in P$.

A brute-force algorithm is obviously $\Theta(n^2)$. A divide-and-conquer approach can improve it to $\Theta(n \log n)$. Its subtlety lies, as usual, in the 3rd step: combination of solutions to the sub-problems. As preparation before the divide-and-conquer, we sort the points respectively by x and y coordinates, and note the results as P_x, P_y . The sort process is $\Theta(n \log n)$ using merge sort, thus we can obtain a $\Theta(n \log n)$ algorithm as long as the divide-and-conquer process takes no more than $\Theta(n \log n)$.

The skeleton of the process is shown in Algorithm 2.4. ClosestSplitPair remains to be illustrated. It outputs the "split pair", i.e. one point in Q and the other in R, with minimum distance.

Let \overline{x} represent the largest x coordinate in Q, i.e. in the left half of P. Since we have P_x , \overline{x} can be obtained in O(1) time. Define S_y as points in P with x coordinate inside $[\overline{x} - \delta, \overline{x} + \delta]$, sorted by y coordinate. We have the following lemma.

Lemma 4. Let $p \in Q, q \in R$ be the split pair with $d(p,q) < \delta$. Then we must have

Algorithm 2.4 Closest Pair Searching ClosetPair (P_x, P_y)

input:

A set of n points $P = \{p_1, \dots, p_n\}$ on \mathbb{R}^2 , sorted respectively by x and y coordinates as P_x and P_y

output:

p,q with minimum Euclidean distance

- 1: Let Q be the left half of P and R be right half of P. According to P_x, P_y , form Q_x, Q_y, R_x, R_y , i.e. Q, R sorted by x and y coordinates. $\triangleright \Theta(n)$
- 2: $(p_1, q_1) = \text{ClosestPair}(Q_x, Q_y)$
- 3: $(p_2, q_2) = \text{ClosestPair}(R_x, R_y)$
- 4: $\delta = \min\{d(p_1, q_1), d(p_2, q_2)\}$
- 5: $(p_3, q_3) = \text{ClosetSplitPair}(P_x, P_y, \delta)$ > Should be O(n)
- 6: Return the best among $(p_1, q_1), (p_2, q_2)$ and (p_3, q_3)
 - $p, q \in S_u$;
 - p,q are at most 7 positions away from each other in S_y .

Proof. Let $p(x_1, y_1) \in Q$, $q(x_2, y_2) \in R$, and we have

$$d(p,q) = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2} < \delta.$$

Since \overline{x} is the largest coordinate in Q, we have

$$x_1 \leq \overline{x} \leq x_2$$
.

Thus

$$|x_2 - \overline{x}| = x_2 - \overline{x} \le x_2 - x_1 \le \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2} < \delta,$$

$$|x_1 - \overline{x}| = \overline{x} - x_1 \le x_2 - x_1 \le \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2} < \delta.$$

Which leads to the conclusion

$$x_1, x_2 \in [\overline{x} - \delta, \overline{x} + \delta].$$

This can be directly translated to the first claim of the lemma: $p, q \in S_y$. Figure 2.1 helps to prove the 2nd claim.



Figure 2.1: p, q at most 7 positions away from each other

In Figure 2.1, we draw $8 \delta/2 \times \delta/2$ grids around \overline{x} and $\min\{y_1, y_2\}$. Since $|y_1 - y_2| < d(p, q) < \delta$ and $p, q \in S_y$, we know that p, q must be contained in these grids. On the other hand, each grid can contain at most 1 point, because if a grid contained 2 points, their distance would be smaller than $\sqrt{2}/2\delta$, thus smaller than δ , violating the prerequisite that δ is the minimum distance between a non-split pair. As a result, there can be at most 8 points inside these grids, including p and q. Hence p, q are at most 7 points away from each other.

According to Lemma 4, we finally have the ClosestSplitPair algorithm as shown in Algorithm 2.5.

```
Algorithm 2.5 ClosestSplitPair(P_x, P_y, \delta)
```

```
input:
```

```
P_x, P_y, \delta as defined in Algorithm 2.4. output:
```

```
Split pair p \in Q, q \in R with d(p,q) < \delta, or null if such pair does not exist.

1: Initialize best = \delta, best\_pair = null

2: for i = 1 to |S_y| - 1 do

3: for j = 1 to \min\{7, |S_y| - i\} do

4: Let p, q be i^{th}, (i + j)^{th} points of S_y

5: if d(p,q) < best then

6: best\_pair = p, q, best = d(p,q)
```

2.4 The Master Method

Potentially useful algorithmic ideas often need mathematical analysis to evaluate. The master method is a general recurrence approach to analyze the running time of divide-and-conquer algorithms.

2.4.1 Examples

Recall the integer multiplication problem. Let T(n) represent the maximum number of primitive operations needed to multiply two n-digit integers. The recurrence approach aims at expressing T(n) in terms of running time of recursive calls concerning smaller n. In this specific divide-and-conquer algorithm, we hope to express T(n) as function of T(n/2). A recurrence approach needs a base case. In this problem the base case is trivial: $T(1) \leq a$, in which a is a constant.

For the divide-and-conquer algorithm without Gauss's trick, we have

$$T(n) \le 4 \cdot T(n/2) + O(n). \tag{2.1}$$

When Gauss's trick is applied, we have

$$T(n) = 3 \cdot T(n/2) + O(n).$$
 (2.2)

Merge sort takes $O(n \log n)$ running time. It has the recurrence relation

$$T(n) = 2 \cdot T(n/2) + O(n).$$
 (2.3)

We have no idea how to obtain the running time from these recurrence relations, but it is clear that the rank of the three algorithms in terms of running time is (2.1)>(2.2)>(2.3).

2.4.2 Mathematical Statement

The master method helps to obtain the running time of an algorithm according to its recurrence relation. It assumes that all sub-problems have equal size, thus it's not applicable to the closest pair problem, in which the left and right halves of the points are not guaranteed to have the same number of points. We also assume that the base case is trivial: $T(n) \leq a$ (a is constant) for all sufficiently small n. Consider an algorithm that has the recurrence relation

$$T(n) \le a \cdot T(n/b) + O(n^d),$$

in which a, b, n are constants with clear meanings. a is the number of recursive calls, b is the input size shrinkage factor, and $O(n^d)$ describes the amount of work needed to combine the solutions to the sub-problems. a, b are both larger than 1, while d can be as small as 0. Master method provides the form of T(n) in different cases, as expressed in Theorem 5.

Theorem 5. T(n) can be expressed in big-O notation as follow²:

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

Now let's look at a few examples.

For merge sort algorithm 1.2 with recurrence relation (2.3), we have a = 2, b = 2, d = 1, thus it belongs to case 1 and has running time $O(n \log n)$. Consider binary search, which has the recurrence relation

$$T(n) = T(n/2) + O(1),$$

i.e. a = 1, b = 2, d = 0, hence it is $O(\log n)$.

For the integer multiplication algorithm without Gauss's trick (2.1), we have a=4, b=2, d=1, ending up with case 3. Thus it has time complexity $O(n^2)$, i.e. the divide-and-conquer approach fails to improve the time consumption in comparison with the primary school method.

When we take Gauss's trick into account, i.e. with Karatsuba multiplication algorithm 1.1, in (2.2) we have $a=3,\ b=2,\ d=1$. We are still in case 3 and end up with $O(n^{\log_2 3})$, which is smaller than $O(n^2)$ but larger than $O(n\log n)$.

²If the recurrence relation is written with = rather than \leq , the result will be in Θ notation.

Strassen's algorithm 2.3 for matrix multiplication has the recurrence relation

$$T(n) = 7 \cdot T(n/2) + O(n^2),$$

which leaves us in case 3. Its running time is therefore $O(n^{\log_2 7})$, which is better than $O(n^3)$.

As an illustration of case 2, consider the recurrence relation

$$T(n) \le 2 \cdot T(n/2) + O(n^2).$$

With a = b = d = 2, we are in case 2, and end up with running time $O(n^2)$. In this case, the running time is governed by the work outside the recursive call, i.e. the time spent on combining solutions to the sub-problems dominates the global time consumption.

2.4.3 Proof

We will prove the correctness of the master method in this section. As having been stated above, we assume that the recurrence relation takes the form

- $T(1) \leq c$
- $T(n) < a \cdot T(n/b) + cn^d$

It's fine to use the same constant c in both the base case and the recurrence relation because we are using \leq . In order to make the process less tedious, we also assume that n is a power of b. The argument will be similar to what we did to obtain the running time of merge sort: through analysis on the recursive tree. Note that in this section when we refer to a value of time consumption, we always mean that the actual time consumption is smaller than or equal to this value.

The recursive tree has $\log_b n + 1$ levels, from level 0 (the original problem) to level $\log_b n$ (trivial problem of size 1). At level j, there are in total a^j subproblems, each of size n/b^j . For $j \neq \log_b n$, the time consumption at this level is contributed by the cn^d term:

$$a^{j} \cdot c \cdot \left(\frac{n}{b^{j}}\right)^{d} = c \cdot n^{d} \cdot \left(\frac{a}{b^{d}}\right)^{j}.$$

Summing it up over all levels leads to the result $c \cdot n^d \cdot \sum_{j=0}^{\log_b n-1} \left(\frac{a}{b^d}\right)^j$. At level $\log_b n$, the time consumption is simply the combination of all base cases:

$$c \cdot a^{\log_b n}$$

The total time consumption is thus

$$c \cdot n^d \cdot \sum_{j=0}^{\log_b n - 1} \left(\frac{a}{b^d}\right)^j + c \cdot a^{\log_b n} = c \cdot n^d \cdot \sum_{j=0}^{\log_b n} \left(\frac{a}{b^d}\right)^j \tag{2.4}$$

This leads to classified discussion over the value of $\frac{a}{b^d}$.

1. $a = b^d$. In this case, (2.4) becomes

$$c \cdot n^d(\log_b n + 1) = O(n^d \log_b n)$$

2. $a < b^d$. In this case, (2.4) becomes

$$c \cdot n^d \frac{1 - \left(\frac{a}{b^d}\right)^{\log_b n + 1}}{1 - \frac{a}{b^d}} < \frac{c}{1 - \frac{a}{b^d}} n^d = O(n^d)$$

3. $a > b^d$. In this case, (2.4) becomes

$$c \cdot n^d \frac{\left(\frac{a}{b^d}\right)^{\log_b n + 1} - 1}{\frac{a}{b^d} - 1} < \frac{c}{\frac{a}{b^d} - 1} n^d \frac{a}{b^d} \left(\frac{a}{b^d}\right)^{\log_b n} = O(a^{\log_b n}) = O(n^{\log_b a})$$

Therefore we have completed the proof of the master method.

The essential role that a/b^d plays here comes naturally from the meaning of a, b, d. Each problem produces a sub-problems in the next level. We call a the **rate of sub-problem proliferation, abbr. RSP**. Size of each sub-problem shrinks by b times after each recurrence, and the work load shrinks by b^d times, so we call b^d the **rate of work shrinkage, abbr. RWS**. The three cases of the master method can be interpreted as follow.

- 1. RSP = RWS. The amount of work at each level is cn^d . With totally $\log_b n$ levels, the problem should be $O(n^d \log_b n)$.
- 2. RSP > RWS. The amount of work increases with the recursion level j. The last level dominates the running time, thus the overall running time is proportional to the number of sub-problems (base cases) in the last level. The problem is $O(a^{\log_b n})$.
- 3. RSP < RWS. The amount of work decreases with the recursion level j. The root level dominates the running time, thus the problem is $O(n^d)$.

Chapter 3

Randomized Algorithms

3.1 Quick Sort

3.1.1 Overview

Quick sort is a prevalent sorting algorithm in practice. It is $O(n \log n)$ on average, and it works in place, i.e. extra memory need to carry out the sort is minimal, whereas for merge sort, we need at least O(n) extra memory. The problem is the same as specified for merge sort. Here we assume that all items inside the array are distinct for simplicity.

The key idea of merge sort is **partition the array around a pivot element**. Plenty of deliberation remains for the choice of the pivot element. For the moment we just assume that the first element is used. In a partition, the array is rearranged so that elements smaller than the pivot are put before the pivot, while elements larger than it are put after the pivot. The partition puts the pivot in the correct position. By recursively partition the two sub-arrays on both sides of the pivot, the whole array becomes sorted. As will be revealed later, a partition can be finished with O(n) time and no extra memory. The skeleton of the algorithm is shown in Algorithm 3.1.

3.1.2 Partition Subroutine

If the in place requirement is thrown away, it is easy to come up with a partition algorithm using O(n) time and O(n) extra memory, as shown in Algorithm 3.2.

Now we try to implement an in-place partition algorithm that uses no extra memory. During the process, the array will be composed of 4 consecutive parts: the pivot p at the first position, then elements smaller than p, elements larger than p and finally elements remaining to be partitioned. Algorithm 3.3 provides such an implementation. It completes the partition in one scan of the array, and uses no extra memory. i is the index of the first element larger than p^1 ,

 $^{^{1}}$ If A[2] is smaller than p, i will not have the same meaning when it gets initialized to 2.

Algorithm 3.1 Skeleton of Quick Sort

input:

Array A with n distinct elements in any order

output:

```
Array A in sorted order

1: if A.len == 1 then

2: return

3: else

4: p = \text{ChoosePivot}(A)

5: Partition A around p

6: Recursively sort 1st part(on left of p)

7: Recursively sort 2nd part(on right of p)
```

Algorithm 3.2 Partition with O(n) Extra Memory

input:

Array A with n(n > 1) distinct elements in any order Pivot element p, put at first position of A

output:

```
Array A partitioned around p

1: Allocate temp[n]

2: small = 1, big = n

3: \mathbf{for} \ i = 2 \ \mathbf{to} \ n \ \mathbf{do}

4: \mathbf{if} \ A[i] > p \ \mathbf{then}

5: temp[big - -] = A[i]

6: \mathbf{else}

7: temp[small + +] = A[i]

8: Assert small == big

9: temp[small] = p

10: Copy temp back to A
```

while j is the index of the first unpartitioned element.

3.1.3 Choice of Pivot

The running time of quick sort depends on the choice of the pivot. The naive approach taken above to always choose the first element is not satisfactory. If the array is already sorted, each time the size of the problem is only reduced by 1, which is no better than selection sort, and the running time if $O(n^2)$. This is indeed the worst case of quick sort. On the contrary, if each time the pivot divides the array into sub-arrays of the same size, we will have the recurrence

But the algorithm is still correct. In such case, i remains the same as j until we encounter the first element larger than p, and swap will not do anything because k and i are always the same when we do the comparison.

Algorithm 3.3 Partition with No Extra Memory

input:

Array A with n(n > 1) distinct elements in any order Pivot element p, put at first position of A

output:

```
Array A partitioned around p

1: i = 2, j = 2

2: for k = 2 to n do

3: if A[k] < p then

4: swap(A[k], A[i++])

5: j + +

6: swap(A[1], A[i-1])
```

relation

$$T(n) = 2 \cdot T(n/2) + O(n),$$

and the running time will be $O(n \log n)$ according to the master method, which is the best case.

3.1.4 Quick Sort Theorem

A good solution is to choose the pivot randomly at every recursive call. We will prove the quick sort theorem 6.

Theorem 6. For every input array A of length n, the average running time of quick sort (with random pivots) is $O(n \log n)$.

The proof of the theorem involves some basic probability knowledge that won't be covered here. Let Ω represent the sample space of all possible sequences of pivots in quick sort. For any $\sigma \in \Omega$, let $C(\sigma)$ represent the number of comparisons between array elements made by quick sort. We have Lemma 7.

Lemma 7. The running time of quick sort is dominated by comparisons, i.e. \exists constant c such that $\forall \sigma \in \Omega$,

$$RT(\sigma) < c \cdot C(\sigma)$$
.

Lemma 7 means that in order to prove the quick sort algorithm, all we need is to prove the expectation of $C(\sigma)$ is $O(n \log n)$. We cannot apply the master method here because in quick sort, the two sub-problems are unlikely to have the same size.

For a fixed input array A, let z_i represent its i^{th} smallest element. Let $x_{ij}(\sigma)$ represent the number of comparisons between z_i and z_j made during quick sort with pivot sequence σ . Whenever a comparison happens, one of the two elements being compared is the pivot. If z_i and z_j have been partitioned respectively into two sides of a pivot before neither is used as pivot, they will never be compared

in the future. If z_i is used as pivot and is compared against z_j , z_i will be at its correct position at the end of the partition, and is excluded from any further comparisons. Thus $\forall i, j, \sigma$, it is clear that $x_{ij}(\sigma)$ is either 0 or 1. A random variable that can only take values 0 and 1, like x_{ij} here, is called an **indicator**.

 $C(\sigma)$ can be expressed as the sum over all x_{ij} :

$$C(\sigma) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} x_{ij}(\sigma).$$

According to the **linearity of expectation**, an taking into account of the fact that x_{ij} is an indicator, we have

$$E[C] = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} E[x_{ij}] = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} P[x_{ij} = 1].$$

Here we are actually applying a **decomposition approach** that goes for the analysis of average running time of a lot of randomized algorithms.

- 1. Identify random variable Y that we care about.
- 2. Express Y as the sum of a series of indicators: $Y = \sum_{l} x_{l}$.
- 3. Apply linearity of expectation: $E[Y] = \sum_{l} E[x_{l}] = \sum_{l} P[x_{l} = 1]$.

It can be proved that for any i < j,

$$P(x_{ij} = 1) = \frac{2}{j - i + 1}$$

Proof. Consider the set of elements

$$S_{ij} = \{z_i, z_{i+1}, \dots, z_{j-1}, z_j\}.$$

As long as none of them is chosen as pivot, they will be passed to the same recursive call. If z_i or z_j is the first among them to be chosen as pivot, x_i and x_j will be compared. On the contrary, if any other element is chosen as pivot before z_i and z_j , z_i and z_j will end up in different sub-arrays, and they can never be compared in the future. So $P(x_{ij} = 1)$ is equal to the probability that z_i or z_j is the first element of S_{ij} to be chosen as pivot, i.e. $\frac{2}{2-i+1}$.

Then we have

$$E[C] = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} P[x_{ij} = 1] = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{2}{j-i+1}$$
$$= 2 \cdot \sum_{i=1}^{n-1} \left(\frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{n-i+1}\right)$$

$$= 2 \cdot \left(\frac{n}{2} + \frac{n-1}{3} + \frac{n-2}{4} + \dots + \frac{1}{n}\right)$$

$$\leq 2n \sum_{k=2}^{n} \frac{1}{k}$$

$$\leq 2n \int_{1}^{n} \frac{1}{x} dx = 2n \ln n$$

Thus the running time of quick sort with random pivots is $O(n \log n)$.

3.2 Randomized Selection

3.2.1 RSelect Algorithm

In this section we will discuss the selection problem.

Input Array A containing n distinct numbers in arbitrary order, and number $i \in \{1, 2, ..., n\}$.

Output The i^{th} order statistic, i.e. i^{th} smallest element of A.

Obviously, the i^{th} order statistic can be found by sorting the array and then directly pick the i^{th} element. The overall running time is at least $O(n \log n)$. A randomized approach similar to that of quick sort can reduce the average running time to O(n), which is quite amazing because simply reading all elements of the array is already an O(n) process. The algorithm is provided in Algorithm 3.4.

Algorithm 3.4 Randomized Selection

```
Array A with n distinct elements in any order
    Integer i \in \{1, 2, ..., n\}
output:
    i^{th} order statistic of A
 1: function RSelect(A, i)
        if A.len == 1 then
 2:
           return A[1]
 3:
        Randomly choose pivot p from A
 4:
        Partition A around p
 5:
        Let j = \text{new index of } p, A_1, A_2 = 1\text{st and 2nd part of } A
 6:
        if j == i then
 7:
           return p
 8:
        else if j > i then
 9:
                                                                     \triangleright A_1.len = j-1
           return RSelect(A_1, i)
10:
        else
11:
                                                 \triangleright j < i. A_2.len = n - j
           return RSelect(A_2, i - j)
12:
```

3.2.2 Running Time

RSelect is also based on recursively partitioning the arrays, but at most one recursive call is needed in each iteration because the i^{th} order statistic can only be on one side of the pivot. As with quick sort, the worse case happens when each time the smallest element is chosen as pivot. The worst running time is $O(n^2)$. The average running time is given by Theorem 8.

Theorem 8. For any input array A of length n, the average running time of RSelect is O(n).

In RSelect, the only workload outside of the recursive call is the partition, which is an O(n) process. Another way to note its time complexity is that it uses fewer than cn operations, in which c is a constant.

Definition 5. RSelect is said to be in phase j if size of the current array is between $(3/4)^{j+1}n$ and $(3/4)^{j}n$.

Let x_j represent the number of recursive calls during phase j. Then we have

$$RT(RSelect) \le cn \sum_{j} x_j \cdot \left(\frac{3}{4}\right)^j$$
 (3.1)

Now let's consider $E(x_j)$. If RSelect chooses a pivot giving a 25%-75% or better partition, the execution is guaranteed to enter the next phase, because the length of the sub-array to examine will shrink by at least 25%. The probability for such a partition to happen is obviously 50%. The problem is analogous to the coin flipping problem. The expectation of x_j is the same as the expectation of the number of flips needed to have the "head" side of the coin show up for the first time. The coin flipping problem is a geometric distribution problem, in which the expectation is $\frac{1}{p} = \frac{1}{1/2} = 2$. Thus $E(x_j) = 2$. Substitute this into (3.1), we have

$$E(RT(RSelect)) \le cn \sum_{j} E(x_j) \left(\frac{3}{4}\right)^j = 2cn \sum_{j} \left(\frac{3}{4}\right)^j \le 8cn.$$

3.3 Deterministic Selection

In this section we will cover a deterministic selection algorithm that is also O(n). It is not a good choice when compared against random selection because the constant for the big-O notation is larger, and it is not in place. Yet it is still a brilliant and interesting algorithm.

When partitioning an array, the ideal pivot is its median. In order to guarantee the efficiency of the algorithm, we need to find a good enough pivot. The key idea is to use the "median of medians". The array is broken into n/5 sub-arrays of length 5. The sub-arrays are sorted, their medians are put into a new array C, and we recursively compute the median of C. The final result is returned as

Algorithm 3.5 Deterministic Selection

```
input:
    Array A with n distinct elements in any order
    Integer i \in \{1, 2, \dots, n\}
output:
    i^{th} order statistic of A
 1: function DSelect(A, i)
 2:
        n = A.len
        if n \leq 5 then
 3:
            sort A and pick the i^{th} element
 4:
        Break A into n/5 sub-arrays of length 5 and sort each sub-array \triangleright O(n)
 5:
        Let array C store the medians of the n/5 sub-arrays
 6:
        p = DSelect(C, n/10)
                                             \triangleright Recursively compute median. T(n/5)
 7:
        Partition A around p
                                                                                  \triangleright O(n)
 8:
        Let j = \text{new index of } p, A_1, A_2 = 1\text{st and 2nd part of } A
 9:
        if j == i then
10:
            return p
11:
        else if j > i then
12:
            return DSelect(A_1, i)
                                              \triangleright T(?) running time to be determined
13:
14:
        else
            return DSelect(A_2, i - j)
15:
```

the pivot. The algorithm is shown in Algorithm 3.5. Two recursive calls are made in Algorithm 3.5. Let T(n) represent the running time of DSelect on an array of length n, then there exists constant c such that

```
    T(1) = 1
    T(n) ≤ cn + T(n/5) + T(?)
```

in which the running time of the second recursive call needs to be determined.

Lemma 9. The 2nd recursive call (line 13 or 15) is guaranteed to be $O(\frac{7}{10}n)$.

Proof. Let k = n/5, and let x_i represent the i^{th} smallest of the k medians. Then the final pivot is $x_{k/2}$. Our goal is to prove that at least 30% of the elements in the input array are smaller than the $x_{k/2}$, and at least 30% are bigger than it. Let's put all elements of the array in a 2D grid as follow, with each sorted group as a column, and x_i in ascending order.

Obviously, elements in red color are smaller than $x_{k/2}$, while elements in blue color are bigger than it. Both include $\frac{3}{5} \times \frac{1}{2} = 30\%$ of the elements. Thus the size of the sub-array is guaranteed to shrink by at least 30% in the 2nd recursive call, so its running time is $O(\frac{7}{10}n)$.

Theorem 10. \forall input array of size n, DSelect runs in O(n) time.

Proof. Now we have

$$T(n) \le cn + T\left(\frac{n}{5}\right) + T\left(\frac{7n}{10}\right).$$

The master method is not applicable because the two sub-problems are not of the same size. We will prove $T(n) \leq 10cn$ by induction.

The base case (n = 1) is trivial. Suppose that $T(k) \leq 10ck$ holds for all k < n. Then we have

$$T(n) \le cn + T\left(\frac{n}{5}\right) + T\left(\frac{7n}{10}\right)$$
$$\le cn + 10c \cdot \frac{n}{5} + 10c \cdot \frac{7n}{10}$$
$$= 10cn$$

Hence T(n) is O(n).

3.4 Lower Bound for Comparison-Based Sorting

Up to now we have in our toolbox $O(n \log n)$ sorting algorithms and O(n) selection algorithms. In this section we will prove that we cannot do better with comparison-based sorting.

Definition 6. In a comparison-based sorting, the array elements can only be accessed via comparisons.

Merge sort, heap sort, quick sort, selection sort are all examples of comparison-based sorting. Bucket sort, counting sort, radix sort are examples of non-comparison-based sorting. They require extra knowledge of the data to sort.

The following theorem provides a lower bound for the running time of comparison-based sorting.

Theorem 11. Every comparison-based sorting algorithm has worst-case running time $\Omega(n \log n)$.

Proof. Consider the action of a comparison-based sorting algorithm on an input composed of integers from 1 to n. There are totally n! such inputs. Let k be the minimum number of comparisons needed to address all these inputs. Each comparison has two possible results, thus k comparisons have 2^k possible

combinations of results. In order for all the n! possible inputs to be sorted correctly, we must have

$$2^k \le n!$$

because otherwise there would be at least 2 inputs that appeared the same for the comparison-based algorithm, according to the pigeonhole principle². Hence we have

$$k \le \log(n!) < \log(n/2)^{n/2} = \frac{n}{2} \log \frac{n}{2},$$

which means that the running time of the algorithm is $\Omega(n \log n)$.

²Also named drawer principle

Chapter 4

Graph Algorithms

Graphs represent pairwise relationships amongst a set of objects. The objects are called vertices or nodes. The relationships are called edges or arcs, each connecting a pair of vertices. An edge can be directed or undirected. The set of vertices and the set of edges are noted respectively as V and E. Graph is a concept heavily used in reality. Road networks, the web, social networks, precedence constraints are all examples of graphs.

A connected graph composed of n vertices with no parallel edges has at least n-1 and at most n(n-1)/2 edges. Let m represent the number of edges. In most applications, m is $\Omega(n)$ and $O(n^2)$. If m is O(n) or close to it, the graph is called a sparse graph, while if m is closer to $O(n^2)$, it's called a dense graph. Yet their delimitation is not strictly clear.

4.1 Representation

4.1.1 Adjacent Matrix

An undirected graph G with n vertices and no parallel edges can be represented by an $n \times n$ 0-1 matrix A. $A_{ij} = 1$ when and only when G has an i - j edge. Variants of this representation can easily accommodate parallel edges, weighted edges: just let A_{ij} represent the number of parallel edges or the weight of the edge. For directed graphs, $i \to j$ can be represented by $A_{ij} = 1$ and $A_{ii} = -1$.

Adjacent matrix representation requires $\Theta(n^2)$ space. For a dense graph this is fine, but for a sparse graph it is wasteful.

4.1.2 Adjacent Lists

The adjacent lists representation is composed of 4 ingredients:

- Array/List of vertices. $\Theta(n)$ space.
- Array/List of edges. $\Theta(m)$ space.

- Each edge points to its end points. $\Theta(m)$ space.
- Each vertex points to edges incident on it. $\Theta(m)$ space.

Adjacent lists representation requires $\Theta(n+m)$ space.

The choice between the two representations depends on the density of the graph and operations to take. We will mainly use adjacent lists in this chapter.

4.2 Minimum Cut

4.2.1 Definition

Definition 7. A cut of a graph (V, E) is a partition of V into two non-empty sets A and B.

A graph with n vertices has $2^n - 2$ possible cuts.

Definition 8. The crossing edges of a cut(A, B) are those with

- one endpoint in A and the other in B, for undirected graphs;
- tail in A and head in B, for directed graphs.

We will try to solve the minimum cut problem:

Input An undirected graph G = (V, E) in which parallel edges are allowed.

Output A cut (A, B) with minimum number of crossing edges.

A lot of problems in reality can be reduced to a minimum cut problems:

- Identify weakness point of physical networks;
- Community detection in social networks;
- Image segmentation.

4.2.2 Random Contraction Algorithm

Algorithm 4.1 provides a random approach to find a cut.

4.2.3 Probability of Correctness

Algorithm 4.1 is not guaranteed to always return a minimum cut. We have to iterate the whole algorithm multiple times and choose the cut with minimum number of crossing edges obtained during the process. In order to estimate the number of iterations needed, we will calculate the probability that a specific minimum cut (A,B) is returned in one iteration.

If one of the crossing edges of (A, B) is selected in step 2, the minimum cut cannot be returned. If there are k crossing edges in (A, B), the probability that

Algorithm 4.1 Random Contraction

input:

An undirected graph G=(V,E) in which parallel edges are allowed. **output:**

A cut (A, B) with minimum number of crossing edges

- 1: while There are more than 2 vertices left do
- 2: Pick a remaining edge (u, v) randomly
- 3: Merge(or contract) u, v into a single vertex
- 4: Remove self-loops
- 5: Return cut represented by 2 final vertices

a crossing edge is selected at the first iteration is k/m. The number of edges decrease by an indefinite number at each iteration, while the number of vertices decrease by exactly 1 each time. Thus it is preferable to express the probability in terms of n instead of m.

Each vertex v is related to a cut (v, V - v). The number of crossing edges of this cut is the number of edges incident on v, i.e. the degree of v. Considering the definition of minimum cut, this number must be larger than k. We also know the sum of the degrees of all vertices: $\sum_{v} degree(v) = 2m$. Thus we have $2m = \sum_{v} degree(v) \ge kn$. Hence the probability that a crossing edge is not selected at the first iteration in step 2 is

$$1 - k/m \ge 2/n.$$

At the second iteration, the same argument still holds. Let m' represent the number of remaining edges after the first iteration. We have $2m' = \sum_{v} degree(v) \ge k(n-1)$. Thus the probability that a crossing edge is selected at the 2nd iteration under the condition that no crossing edge was selected at the 1st iteration is

$$1 - k/m' > 2/(n-1)$$

The same argument continues further until the last iteration, i.e. the $(n-2)^{th}$ iteration. Finally, the probability that no crossing edge is selected in the whole process, thus resulting in the minimum cut (A, B) is

$$P(A,B) \ge \left(1 - \frac{2}{n}\right) \left(1 - \frac{2}{n-1}\right) \cdots \left(1 - \frac{2}{n-(n-3)}\right)$$
$$= \frac{(n-2) \cdot (n-3) \cdots 2 \cdot 1}{n \cdot (n-1) \cdots 4 \cdot 3}$$
$$= \frac{2}{n(n-1)} > \frac{1}{n^2}.$$

The probability seems small, but it already makes great advancement when compared with brute-force method, in which case the probability to obtain (A, B) in an iteration is $\frac{1}{2^n}$.

After N iterations, the probability that (A, B) has not been found is

$$P(not\ found) < \left(1 - \frac{1}{n^2}\right)^N \le e^{-\frac{N}{n^2}}.$$

If $N=n^2$, the probability is smaller than 1/e. If $N=n^2 \ln n$, it is smaller than 1/n.

4.2.4 Number of Minimum Cuts

A graph can have multiple minimum cuts. For example, a tree with n vertices has n-1 minimum cuts. We would like to find the largest number of minimum cuts that a graph with n vertices can have.

Theorem 12. A graph with n vertices can have at most $\binom{n}{2}$ minimum cuts.

Proof. Consider the graph in which the n vertices form a circle. Removing any two edges results in a minimum cut. Thus in total it has $\binom{n}{2}$ minimum cuts. The rest of the proof aims at proving that a graph with n vertices cannot have more minimum cuts.

Recall that the probability for Algorithm 4.1 to return a specific minimum cut is bigger than $\frac{2}{n(n-1)}$. Suppose there are k minimum cuts. The events "Algorithm 4.1 returns minimum cut C_i " and "Algorithm 4.1 returns minimum cut C_j " are disjoint events when $i \neq j$. Thus we have

$$1 \ge P(\text{return a minimum cut}) \ge \frac{2k}{n(n-1)}.$$

Therefore,

$$k \le \frac{n(n-1)}{2} = \binom{n}{2}.$$

4.3 Breadth First Search

Graph search is widely used for various purposes:

- Check if a network is connected;
- Find shortest paths, e.g. for driving navigation, or formulating a plan;
- Calculate connected components.

• ...

We will introduce a few fast algorithms based on graph search. Graph search usually starts from a source vertex. When searching the graph, we want to find everything that is findable, i.e. every vertex reachable from the source via a path. Moreover, we never explore anything twice. In terms of running time, our goal is O(m+n).

BFS explores the nodes of a graph in layers. Nodes with the same distances from the source are in the same layer. It can be used to compute shortest paths of graphs, and to compute connected components of undirected graphs. It guarantees O(m+n) running time. The general pattern of BFS is shown in Algorithm 4.2.

Algorithm 4.2 Breadth First Search(BFS)

input:

Graph G with all vertices unexplored Source vertex s

output:

G with all vertices reachable from s explored.

- 1: Mark s as explored.
- 2: Let Q = queue initialized with s
- 3: while $Q \neq \emptyset$ do
- 4: Remove first element v of Q
- 5: **for** each edge (v, w) **do**
- 6: **if** w is unexplored **then**
- 7: Mark w as explored
- 8: Add w to Q

At the end of BFS, the fact that a node v is explored means the existence of a path from s to v.

4.3.1 Shortest Path

Algorithm 4.3 calculates the shortest path from s to any vertex reachable from s.

After the algorithm terminates, dist(v) = i means that v is in the ith layer and that the shortest path connecting s and v has i edges.

4.3.2 Undirected Connectivity

Definition 9. For an undirected graph G(V, E), connected components are equivalence classes of the equivalence relation¹ $u \sim v$, in which u, v are its vertices and $u \sim v \iff \exists$ path from u to v.

Identifying connected components of graphs is useful for various purposes:

 $^{^1}$ An equivalence relation on a set must satisfy: 1. $a\sim a;$ 2. If $a\sim b,$ then $b\sim a;$ 3. If $a\sim b$ and $b\sim c,$ then $a\sim c.$

Algorithm 4.3 Shortest Path - BFS

input:

Graph G with all vertices unexplored Source vertex s

output:

```
dist(v) for any vertex v, i.e. min number of edges on a path from s to v
 1: Initialize dist(v) = \begin{cases} 0, & if(v == s) \\ +\infty, & if(v \neq s) \end{cases}
 2: Mark s as explored.
 3: Let Q = queue initialized with s
 4: while Q \neq \emptyset do
        Remove first element v of Q
        for each edge (v, w) do
 6:
 7:
            if w is unexplored then
                Mark w as explored
 8:
                dist(w) = dist(v) + 1
 9:
10:
                Add w to Q
```

- Check if a network is disconnected;
- Graph visualization;
- Clustering.

When it comes to the calculation of connected component, undirected graphs and directed graphs are significantly different. BFS is an effective method for calculating the connectivity of undirected graphs. Algorithm 4.4 computes the CCs of an undirected graph in O(m+n) time.

Algorithm 4.4 Connected Components of Undirected Graph - BFS

input:

Undirected graph G with all vertices unexplored and labeled 1 to noutput:

```
Connected components of G
1: for i = 1 to n do
      if i not explored then
          BFS(G,i)
                                            \triangleright discovers i's connected component
3:
```

Depth First Search 4.4

DFS is a more aggressive method to search an graph than BFS. It explores the nodes following the edges as deeply as possible, and only backtracks when necessary. DFS is especially important for dealing with directed graphs. As we are about to demonstrate, it helps to compute topological ordering of directed acyclic graphs and strongly connected components of directed graphs. As with BFS, DFS also runs in O(m+n) time.

DFS can be implemented by mimicking BFS in Algorithm 4.2. A stack should be used instead of a queue. A recursive approach is shown in Algorithm 4.5. DFS can also be used to calculate connected components of undirected

Algorithm 4.5 Depth First Search (Recursive)

input:

Graph G with all vertices unexplored Source vertex s

output:

G with all vertices reachable from s explored.

```
1: function DFS(Graph G, node s)
```

- 2: Mark s as explored
- 3: **for** each edge (s, v) **do**
- 4: **if** v not explored **then**
- 5: DFS(G, v)

graphs. But we will focus on two applications of DFS that cannot be handled with BFS.

4.4.1 Topological Sort

Topological sort aims at putting the nodes of a directed graph in topological ordering.

Definition 10. A topological ordering of a directed graph G is a labeling f of G's nodes among $\{1, 2, ..., n\}$ such that $\forall (u, v) \in G$, f(u) < f(v).

All edges of a directed graph go forward in a topological ordering. Topological sort is applied when the order of a sequence of tasks with precedence constraints needs to be arranged. Note that if a directed graph contains a cycle, there exists no topological ordering for it. This condition is actually necessary and sufficient.

Theorem 13. A directed graph has a topological ordering if and only if it contains no cycle.

One way to find a topological ordering of a DAG is by identifying sink nodes, i.e. nodes with no outgoing arcs.

Theorem 14. A DAG has at least one sink node.

Proof. The theorem can be proved by contradiction easily. Suppose we have a DAG containing no sink node. Starting from a source node, we can follow one of its outgoing arcs to a new node. The process can be done indefinitely because

every node has outgoing arcs. But it is inevitable that at least one node will be visited multiple times after n+1 steps, forming a cycle, which contradicts with the definition of DAG.

A sink node is a perfect candidate for the last position in the topological ordering: no arc starts from it. Algorithm 4.6 calculates the topological ordering of a DAG by recursively putting a sink node at the end of the ordering.

Algorithm 4.6 Topological Ordering of DAG

input:

Directed acyclic graph G with n nodes

output:

```
Topological ordering of G
1: function TopologicalOrdering(Graph G)
     if G is empty then
2:
         return
3:
     Find a sink node v in G
4:
5:
     set f(v) = n
     TopologicalOrdering(G - \{v\})
6:
```

The algorithm using DFS is shown in Algorithm 4.7. A loop over the nodes is added in order to guarantee the correctness when G is not connected.

Algorithm 4.7 Topological Ordering of DAG - DFS

input:

Directed acyclic graph G with n nodes, unexplored output:

```
Topological ordering of G
 1: function DFSLoop(Graph G)
 2:
      current\_label = n
      for each v in G do
3:
          if v not explored then
 4:
             DFS(G,v)
 5:
 6: function DFS(Graph G, node s)
      Mark s as explored
 7:
      for each edge (s, v) do
8:
          if v not explored then
 9:
             DFS(G,v)
10:
      f(s) = current\_label - -
11:
```

Strongly Connected Components 4.4.2

The concept of connectivity in directed graphs is different from that in undirected graphs.

Definition 11. Strong connected components (SCCs) of a directed graph G(V, E) are equivalence classes of the equivalence relation $u \sim v$, in which $u, v \in V$ and $u \sim v \iff \exists$ path from u to v as well as from v to u.

Algorithm 4.8 computes all SCCs of a directed graph by running DFS twice, thus in O(m+n) time. In the end, vertices with the same "leader" are in the same SCC. An example is provided in Figure 4.1.

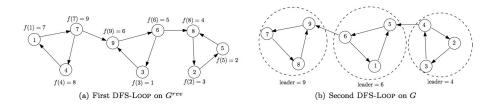


Figure 4.1: Example of Algorithm 4.8

Algorithm 4.8 Kosaraju's 2-Pass SCC Algorithm - DFS input: Directed graph G(V, E) with n nodes labeled 1 to n output: SCCs of G1: Reverse G to get G^{rev} 2: 1^{st} loop: $DFSLoop(G^{rev})$ 3: 2^{nd} loop: DFSLoop(G)4: **function** DFSLoop(Graph G) Set all nodes unexplored 5: $t \coloneqq 0, s \coloneqq null$ $\triangleright t$: finish time. s: current leader 6: 2^{nd} loop only: Relabel nodes according to f(i)7: for i = n to 1 do 8: if i not explored then 9: 2^{nd} loop only: s := i10: DFS(G, i)11: 12: **function** DFS(Graph G, node i)Mark i as explored 13: 2^{nd} loop only: leader(i) := s14: for each arc $i \to j \in E$ do 15: if j not explored then 16: DFS(G, j)17: 1^{st} loop only: f(i) := + + t18:

The SCCs of a directed graph induce a meta-DAG. The meta-nodes are the SCCs, while its arcs are the original arcs between different SCCs, as shown in

Figure 4.2. It is guaranteed to be a DAG because the existence of any loop in the meta-graph will force a few SCCs to collapse into one big SCC.

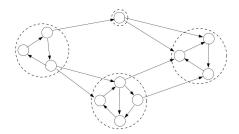


Figure 4.2: Meta-graph induced by SCCs

DFS from a node is guaranteed to reach all other nodes in the same SCC, but it will also reach other SCCs as long as there exist outgoing arcs from this SCC, which are also outgoing arcs in the meta-DAG. Sink nodes in the meta-DAG do not have outgoing arcs, thus the correspondent SCC can be isolated if we start a DFS from one node in this SCC. Algorithm 4.8 does exactly this. In order to prove its correctness we need the following lemma.

Lemma 15. Consider two adjacent SCCs of $G: C_1$ and C_2 such that \exists arc $i \rightarrow j$ in which $i \in C_1$, $j \in C_2$. Let f(v) denote the finishing time determined in the 1st loop of Algorithm 4.8 for node v. Then we must have

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

Proof. In G^{rev} , there exists arc $j \to i$. Let v represent the first vertex in $C_1 \cup C_2$ to be explored. v can be in either C_1 or C_2 , as shown in Figure 4.3.

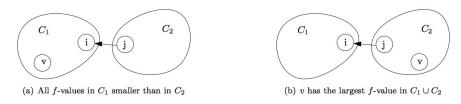


Figure 4.3: Proof of Lemma 15

If $v \in C_1$, then none of the nodes in C_2 will be explored before all nodes in C_1 are explored, because there exists no arc from C_1 to C_2 . Thus we have $f(v_1) < f(v_2)$, $\forall v_1 \in C_1, v_2 \in C_2$, which is a stronger conclusion than our original argument in the lemma.

If $v \in C_2$, DFS for v won't finish before DFSs for all nodes in C_2 finish. In particular, DFS for j won't finish before DFS for all nodes in C_1 finish. Hence

v will have the largest f value amongst all nodes in $C_1 \cup C_2$, and we have $f(v) = \max_{i \in C_2} f(i) > \max_{i \in C_1} f(i)$

An obvious corollary of Lemma 15 is as follow.

Corollary 16. $\max_{v \in V} f(v)$ must lie in a sink SCC, i.e. an SCC that has no outgoing arc.

Therefore, by starting from the node with the largest f value in the 2^{nd} loop, we are guaranteed to explore a sink SCC of G first. Nodes in this sink SCC are ruled out from further exploration because there have been marked as explored. Every time we set up a new leader, it is guaranteed to be the node with the largest f value amongst all unexplored nodes. DFS from the leader will reach and will only reach nodes in the same SCC as the leader, which is a sink SCC of the unexplored part of the graph. The SCCs will be found one by one.

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