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Algorithms and Data Structures

The Basic Toolbox

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Preface

Algorithms are at the heart of every nontrivial computer application. Therefore every computer scientist and every professional programmer should know about the basic algorithmic toolbox: structures that allow efficient organization and retrieval of data, frequently used algorithms, and basic techniques for modeling, understanding, and solving algorithmic problems.

This book is a concise introduction to this basic toolbox intended for students and professionals familiar with programming and basic mathematical language. We have used sections of the book for advanced undergraduate lectures on algorithmics and as the basis for a beginning graduate level algorithms course. We believe that a concise yet clear and simple presentation makes the material more accessible as long as it includes examples, pictures, informal explanations, exercises, and some linkage to the real world.

Most chapters have the same basic structure. We begin by discussing the problem adressed as it occurs in a real-life situation. We illustrate the most important applications and then introduce simple solutions *as informally as possible and as formally as necessary* to really understand the issues at hand. When moving to more advanced and optional issues, this approach logically leads to a more mathematical treatment including theorems and proofs. Advanced sections, that can be skipped on first reading are marked with a star*. Exercises provide additional examples, alternative approaches and opportunities to think about the problems. It is highly recommended to have a look at the exercises even if there is no time to solve them during the first reading. In order to be able to concentrate on ideas rather than programming details, we use pictures, words, and high level pseudocode for explaining our algorithms. A section with implementation notes links these abstract ideas to clean, efficient implementations in real programming languages such as C++ or Java. [C-sharp]Each ⟸ chapter ends with a section on further findings that provides a glimpse at the state of research, generalizations, and advanced solutions.

Algorithmics is a modern and active area of computer science, even at the level of the basic tool box. We made sure that we present algorithms in a modern way, including explicitly formulated invariants. We also discuss recent trends, such as algorithm engineering, memory hierarchies, algorithm libraries, and certifying algorithms.

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October, 2007 *Peter Sanders*

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[amuse geule arithmetik. Bild von Al Chawarizmi] ⟸

1

Appetizer: Integer Arithmetics

Fig. 1.1. *Al-Khwarizmi* (born approx. 780; died between 835 and 850), Persian mathematician and astronomer from the *Khorasan* province of todays Uzbekistan. The word ‘algorithm’ is derived from his name.

[Bild oben wie in anderen Kapiteln?] An appetizer is supposed to stimulate the appetite at the beginning of a meal. This is exactly the purpose of this chapter. We want to stimulate your interest in algorithmic techniques by showing you a first surprising result. The school method for multiplying integers is not the best multiplication algorithm; there are much faster ways to multiply large integers, i.e., integers with thousands and even million of digits, and we will teach you one of them. ⟸

Arithmetic on long integers is needed in areas such as cryptography, geometric computing, and computer algebra and so the improved multiplication algorithm is not just an intellectual gem but also useful for applications.

On the way, we will learn basic analysis and basic algorithm engineering techniques in a simple setting. We will also see the interplay of theory and experiment.

We assume that integers are represented as digit strings. In the base B number system, where B is an integer larger than one, there are digits 0, 1, to $B-1$ and a digit string $a_{n-1}a_{n-2}\ldots a_1a_0$ represents the number $\sum_{0\le i<n} a_iB^i$. The most important systems with a small value of B are base 2 with digits 0 and 1, base 10 with digits 0 to 9, and base 16 with digits 0 to 15 (frequently written as 0 to 9, A, B, C, D, E, F). Larger bases, such as 2^8, 2^{16}, 2^{32}, and 2^{64}, are also useful. We have

$$\begin{aligned}
\text{"10101" in base 2 represents} \quad & 1\cdot 2^4+0\cdot 2^3+1\cdot 2^2+0\cdot 2^1+1\cdot 2^0 = && 21\\
\text{"924" in base 10 represents} \quad & 9\cdot 10^2+2\cdot 2\cdot 10^1+4\cdot 10^0 = && 924\,.
\end{aligned}$$

We assume that we have two primitive operations at our disposal: the addition of three digits with a two digit result (this is sometimes called a full adder) and the multiplication of two digits with a two digit result[1]. For example, in base 10, we have

$$\begin{array}{r} 3 \\ 5 \\ 5 \\ \hline 13 \end{array} \qquad \text{and} \qquad 6 \cdot 7 = 42 \,.$$

We will measure the efficiency of our algorithms by the number of primitive operations executed.

We can artificially turn any n-digit integer into an m-digit integer for any $m \geq n$ by adding additional leading zeroes. Concretely, "425" and "000425" represent the same integer. We will use a and b for the two operands of an addition or multiplication and assume throughout this section that a and b are n-digit integers. The assumption that both operands have the same length simplifies presentation without changing the key message of the chapter. We come back to this remark at the end of the chapter. We refer to the digits of a as a_{n-1} to a_0 with a_{n-1} being the most significant (also called leading) digit and a_0 being the least significant digit and write $a = (a_{n-1} \ldots a_0)$. The leading digit may be zero. Similarly, we use b_{n-1} to b_0 to denote the digits of b and write $b = (b_{n-1} \ldots b_0)$.

1.1 Addition

We all know how to add two integers $a = (a_{n-1} \ldots a_0)$ and $b = (b_{n-1} \ldots b_0)$. We simply write one under the other with the least significant digits aligned and sum digit-wise, carrying a single digit from one position to the next. The result will be an $n+1$-digit integer $s = (s_n \ldots s_0)$. Graphically,

$$\begin{array}{rrrrrr} & a_{n-1} & \ldots & a_1 & a_0 & \text{first operand} \\ & b_{n-1} & \ldots & b_1 & b_0 & \text{second operand} \\ c_n & c_{n-1} & \ldots & c_1 & 0 & \text{carries} \\ \hline s_n & s_{n-1} & \ldots & s_1 & s_0 & \text{sum} \end{array}$$

where c_n to c_0 is the sequence of carries and $s = (s_n \ldots s_0)$ is the sum. We have $c_0 = 0$, $c_{i+1} \cdot B + s_i = a_i + b_i + c_i$ for $0 \leq i < n$ and $s_n = c_n$. As a program, this is written as:

```
c = 0 : Digit                                        // Variable for the carry digit
for i := 0 to n − 1 do  add a_i, b_i, and c to form s_i and a new carry c
s_n = c
```

We need one primitive operation for each position and hence a total of n primitive operations.

Theorem 1. *The addition of two n-digit integers requires exactly n primitive operations. The result is an $n+1$-digit integer.*

[1] Observe that the sum of three digits is at most $3(B-1)$ and the product of two digits is at most $(B-1)^2$ and that both expressions are bounded by $(B-1) \cdot B^1 + (B-1) \cdot B^0 = B^2 - 1$, the largest integer that can be written with two digits.

1.2 Multiplication: The School Method

We all know how to multiply two integers. In this section we will review the school method. In a later section we will get to know a method which is significantly faster for large integers.

We will proceed slowly. We first review how to multiply an n-digit integer a by a 1-digit integer b_j. We use b_j for the 1-digit integer since this is how we need it below. For any digit a_i of a we form the product $a_i \cdot b_j$. The result is a two-digit integer $(c_i d_i)$, i.e.,

$$a_i \cdot b_j = c_i \cdot B + d_i \,.$$

We form two integers $c = (c_{n-1} \ldots c_0\, 0)$ and $d = (d_{n-1} \ldots d_0)$ from the c's and d's, respectively. Since the c's are the higher order digits in the products, we add a zero digit at the end. We add c and d to obtain the product $p_j = a \cdot b_j$. Graphically,

$$(a_{n-1} \ldots a_i \ldots a_0) \cdot b_j \quad \longrightarrow \quad \begin{array}{c} c_{n-1}\ c_{n-2}\ \ldots\ c_i \quad c_{i-1}\ \ldots\ c_0\ \ 0 \\ \quad d_{n-1}\ \ldots\ d_{i+1}\ d_i \quad \ldots\ d_1\ d_0 \\ \hline \text{sum of } c \text{ and } d \end{array}$$

Let us determine the number of primitive operations. For each i, we need one primitive operation to form the product $a_i \cdot b_j$, for a total of n primitive operations. Then we add two $n+1$-digit numbers. This requires $n+1$ primitive operations. So the total number of primitive operations is $2n+1$.

Lemma 1. *We can multiply an n-digit number with a 1-digit number with $2n+1$ primitive operations. The result is an $n+1$-digit number.*

When you multiply an n-digit number by a 1-digit number you probably proceed slightly differently. You combine[2] the generation of the products $a_i \cdot b_j$ with the summation of c and d into a single phase, i.e., you create the digits of c and d when they are needed in the final addition. We have chosen to generate them in a separate phase because this simplifies the description of the algorithm.

Exercise 1. Give a program for the multiplication of a and b_j that operates in a single phase.

We can now turn to the multiplication of two n-digit integers. The *school method* for integer multiplication works as follows: we first form partial products p_j by multiplying a with the j-th digit b_j of b and then sum the suitably aligned products $p_j \cdot B^j$ to obtain the product of a and b. Graphically,

$$\begin{array}{r} p_{0,n-1}\ \cdots\ p_{0,2}\ p_{0,1}\ p_{0,0} \\ p_{1,n-1}\ p_{1,n-2}\ \cdots\ p_{1,1}\ p_{1,0} \qquad\quad \\ p_{2,n-1}\ p_{2,n-2}\ p_{2,n-3}\ \cdots\ p_{2,0} \qquad\qquad\quad \\ \cdots \qquad\qquad\quad \\ p_{n-1,n-1}\ \cdots \qquad p_{n-1,1}\ p_{n-1,0} \qquad\qquad\qquad\qquad \\ \hline \text{sum of the } n \text{ partial products} \end{array}$$

[2] In compiler construction and performance optimization literature, this transformation is known as *loop fusion*.

The description in pseudocode is more compact. We initialize the product p to zero and then add to it the partial products $a \cdot b_j \cdot B^j$ one by one.

```
$p = 0$ : ℕ
**for** $j := 0$ **to** $n - 1$ **do** $p := p + a \cdot b_j \cdot B^j$
```

Let us analyze the number of primitive operations required by the school method. Each partial product p_j requires $2n + 1$ primitive operations and hence all partial products require a total of $2n^2 + n$ primitive operations. The product $a \cdot b$ is a $2n$-digit number and hence all summations $p + a \cdot b_j \cdot B^j$ are summations of $2n$-digit integers. Each such addition requires at most $2n$ primitive operations and hence all additions require at most $2n^2$ primitive operations. Thus, we need no more than $4n^2 + n$ primitive operations in total.

A simple observation allows us to improve the bound. The number $a \cdot b_j \cdot B^j$ has $n + 1 + j$ digits, the last j of which are zero. We can therefore start the addition in the $j + 1$-th position. Also, when we add $a \cdot b_j \cdot B^j$ to p, we have $p = a \cdot (b_{j-1} \cdots b_0)$, i.e., p has $n + j$ digits. Thus, the addition of p and $a \cdot b_j \cdot B^j$ amounts to the addition of two $n + 1$ digit numbers and requires only $n + 1$ primitive operations. Therefore, all additions require only $n^2 + n$ primitive operations. We have thus shown:

Theorem 2. *The school method multiplies two n-digit integers with $3n^2 + 2n$ primitive operations.*

We have now analyzed the number of primitive operations required by the school methods for integer addition and integer multiplication. The number M_n of primitive operations for the school method for integer multiplication is $3n^2 + 2n$. Observe that $3n^2 + 2n = n^2(3 + 2/n)$ and hence $3n^2 + 2n$ is essentially the same as $3n^2$ for large n. We say that M_n *grows quadratically*. Observe also that

$$M_n/M_{n/2} = \frac{3n^2 + 2n}{3(n/2)^2 + 2(n/2)} = \frac{n^2(3 + 2/n)}{(n/2)^2(3 + 4/n)} = 4 \cdot \frac{3n + 2}{3n + 4} \approx 4 ,$$

i.e., quadratic growth has the consequence of essentially quadrupling the number of primitive operations when the size of the instance is doubled.

Assume now that we actually implement the multiplication algorithm in our favorite programming language (we will do so later in the chapter) and then time the program on our favorite machine for different n-digit integers a and b and different n. What should we expect? We want to argue that we will see quadratic growth. The reason is that *primitive operations are representative for the running time of the algorithm*. Consider addition of two n-digit integers first. What happens when the program is executed? For each position i, the digits a_i and b_i have to be moved to the processing unit, the sum $a_i + b_i + c$ has to be formed, the digit s_i of the result needs to be stored in memory, the carry c is updated, the index i is incremented and a test for loop exit needs to be performed. Thus for each i, the same number of machine cycles is executed. We counted one primitive operation for each i and hence the number of primitive operations is representative for the number of executed machine cycles. Of course, there are additional effects: for example, pipelining and the complex transport mechanism for data between memory and processing unit, but they will have a similar effect for all i and hence the number of primitive operations is also representative for the running time of an actual implementation on an actual machine. The argument extends to multiplication since multiplication of a number by a 1-digit number is a process similar to addition and since the second phase of the school method for multiplication amounts to a series of additions.

Let us confirm the argument by an experiment. Figure 1.2 shows execution times of a C++ implementation of the school method; the program can be found in Section 1.7. For each n, we performed a large number[3] of multiplications of n-digit random integers and then determined the average running time T_n; T_n is listed in the second column. We also show the ratio $T_n/T_{n/2}$. Figure 1.2 also shows a plot of the data points[4] $(\log n, \log T_n)$. The data exhibits approximately quadratic growth as we can deduce in different ways. The ratio $T_n/T_{n/2}$ is always close to four, and the double logarithmic plot shows essentially a line of slope two. The experiments are quite encouraging: *our theoretical analysis has predictive value. Our theoretical analysis showed quadratic growth of the number of primitive operations, we argued above that actual running time should be related to the number of primitive operations, and the actual running time essentially grows quadratically.* However, we also see systematic deviations. For small n, the growth from one row to the next is less than four, as linear and constant terms in the running time still play a substantial role. For larger n, the ratio is very close to four. For very large n (too large to be timed conveniently), we would probably see a factor larger than four since access time to memory depends on the size of the data. We will come back to this point in Section **??**.

Exercise 2. Write programs for long integer addition and multiplication. Represent integers as sequences (arrays or lists or whatever your programming language offers) of decimal digits and use the built-in arithmetic to implement the primitive operations. Then write the ADD, MULTIPLY1, and MULTIPLY functions that add integers, multiply an integer by a 1-digit number, and multiply integers respectively. Use your implementation to produce your own version of Figure 1.2. Experiment with using a larger base than base 10, say base 2^{16}.

Exercise 3. Describe and analyze the school method for division.

1.3 Result Checking

Our algorithms for addition and multiplication are quite simple and hence it is fair to assume that we can implement them correctly in the programming language of our

[3] The internal clock measuring CPU time returns its timings in some unit, say milliseconds, and hence the required rounding introduces an error of up to one-half of this unit. It is therefore important that the experiment timed takes much longer than this unit, in order to reduce the effect of rounding.

[4] Throughout this book we use $\log x$ to denote the logarithm $\log_2 x$ to base 2.

n	T_n [sec]	$T_n/T_{n/2}$
8	0.00000469	
16	0.0000154	3.28527
32	0.0000567	3.67967
64	0.000222	3.91413
128	0.000860	3.87532
256	0.00347	4.03819
512	0.0138	3.98466
1024	0.0547	3.95623
2048	0.220	4.01923
4096	0.880	4
8192	3.53	4.01136
16384	14.2	4.01416
32768	56.7	4.00212
65536	227	4.00635
131072	910	4.00449

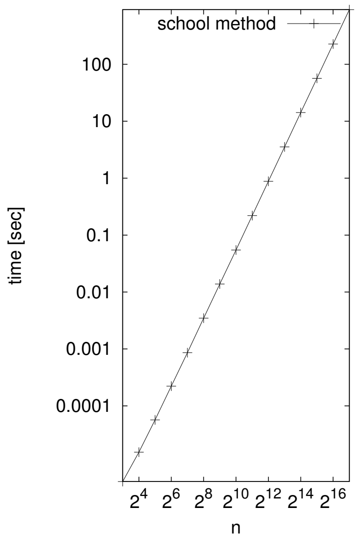


Fig. 1.2. The running time of the school method for the multiplication of n-digit integers. The three columns of the table on the left give n, the running time T_n of the C++ implementation of Section 1.7, and the ratio $T_n/T_{n/2}$. The plot on the right shows $\log T_n$ versus $\log n$ and we see essentially a line. Observe, if $T_n = \alpha n^\beta$ for some constants α and β then $T_n/T_{n/2} = 2^\beta$ and $\log T_n = \beta \log n + \log \alpha$, i.e., $\log T_n$ depends linearly on $\log n$ with slope β. In our case, the slope is two. Please, use a ruler to check.

choice. However, writing software[5] is an error-prone activity and hence we should always ask ourselves whether we can check the results of a computation. For multiplication, the authors were taught the following technique in elementary school. The method is known as *Neunerprobe* in German, *casting out nines* in English, and *preuve par neuf* in French.

Add the digits of a. If the sum is a number with more than one digit, sum its digits. Repeat until you arrive at a one digit number, called the checksum of a. We use s_a to denote it. Here is an example:

$$4528 \rightarrow 19 \rightarrow 10 \rightarrow 1\ .$$

Do the same for b and the result c of the computation. This gives the checksums s_b and s_c. All checksums are single digit numbers. Compute $s_a \cdot s_b$ and form its checksum s. If s differs from s_c, c is not equal to $a \cdot b$. This test was already described by Al-Kwarizmi in his book on algebra.

Let us go through a simple example. Let $a = 429$, $b = 357$, and $c = 154153$. Then $s_a = 6$, $s_b = 6$ and $s_c = 1$. Also $s_a \cdot s_b = 36$ and hence $s = 9$. So $s_c \neq s$ and

[5] The bug in the division algorithm of the floating point unit of the original Pentium chip became famous. It was caused by a few missing entries in a lookup table used by the algorithm.

hence s_c is not the product of a and b. Indeed, the correct product is $c = 153153$. Its checksum is 9 and hence the correct product passes the test. The test is not foolproof, as $c = 135153$ also passes the test. However, the test is quite useful and detects many mistakes.

What is the mathematics behind this test? We explain a more general method. Let q be any positive integer; in the method described above, $q = 9$. Let s_a be the remainder or residue in the integer division a divided by q, i.e. $s_a = a - \lfloor a/q \rfloor \cdot q$. Then[6] $0 \leq s_a < q$. In mathematical notation, $s_a = a \bmod q$. Similarly, $s_b = b \bmod q$ and $s_c = c \bmod q$. Finally, $s = (s_a \cdot s_b) \bmod q$. If $c = a \cdot b$, then it must be the case that $s = s_c$. Thus $s \neq s_c$ proves $c \neq a \cdot b$ and uncovers a mistake in the multiplication. What do we know if $s = s_c$? We know that q divides the difference of c and $a \cdot b$. If this difference is non-zero, the mistake will be detected by any q which does not divide the difference.

Let us continue with our example and take $q = 7$. Then $a \bmod 7 = 2$, $b \bmod 7 = 0$ and hence $s = (2 \cdot 0) \bmod 7 = 0$. But $135153 \bmod 7 = 4$ and we uncovered that $135153 \neq 429 \cdot 357$.

Exercise 4. Explain why the method learned by the authors in school corresponds to the case $q = 9$. Hint: $10^k \bmod 9 = 1$ for all $k \geq 0$.

Exercise 5 (Elferprobe, Casting out Elevens). Powers of ten have very simple reminders modulo 11, namely $10^k \bmod 11 = (-1)^k$ for all $k \geq 0$, i.e., $1 \bmod 11 = 1$, $10 \bmod 11 = -1$, $100 \bmod 11 = +1$, $1000 \bmod 11 = -1$. Describe a simple test to check correctness of a multiplication modulo 11.

1.4 A Recursive Version of the School Method

We will derive a recursive version of the school method. This will be our first encounter of the *divide-and-conquer paradigm*, one of the fundamental paradigms in algorithm design.

Let a and b be our two n-digit integers which we want to multiply. Let $k = \lfloor n/2 \rfloor$. We split a into two numbers a_1 and a_0; a_0 consists of the k least significant digits and a_1 consists of the $n-k$ most significant digits[7]. We split b analogously. Then

$$a = a_1 \cdot B^k + a_0 \quad \text{and} \quad b = b_1 \cdot B^k + b_0$$

and hence

$$a \cdot b = a_1 \cdot b_1 \cdot B^{2k} + (a_1 \cdot b_0 + a_0 \cdot b_1) \cdot B^k + a_0 \cdot b_0 \ .$$

This formula suggests the following algorithm for computing $a \cdot b$:

[6] The method taught in school uses residues 1 to 9 instead of 0 to 8 according to the definition $s_a = a - (\lceil a/q \rceil - 1) \cdot q$

[7] Observe that we changed notation. a_0 and a_1 now denote the two parts of a and are no longer single digits.

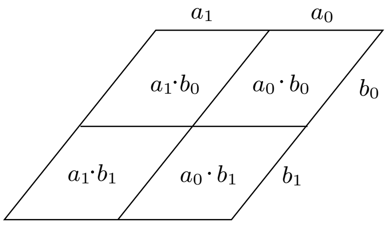


Fig. 1.3. Visualization of the school method and its recursive variant: the rhombus-shaped area indicates the partial products in the multiplication $a \cdot b$. The four sub-areas correspond to the partial products in the multiplications $a_1 \cdot b_1$, $a_1 \cdot b_0$, $a_0 \cdot b_1$, and $a_0 \cdot b_0$, respectively. In the recursive scheme, we first sum the partial products in the four sub-areas and then in a second step add the four resulting sums.

(a) Split a and b into a_1, a_0, b_1, and b_0.
(b) Compute the four products $a_1 \cdot b_1$, $a_1 \cdot b_0$, $a_0 \cdot b_1$, and $a_0 \cdot b_0$.
(c) Add the suitably aligned products to obtain $a \cdot b$.

Observe that the numbers a_1, a_0, b_1, and b_0 are $\lceil n/2 \rceil$-digit numbers and hence the multiplications in step (b) are simpler than the original multiplication if $\lceil n/2 \rceil < n$, i.e., $n > 1$. The complete algorithm is now as follows: to multiply 1-digit numbers, use the multiplication primitive. To multiply n-digit numbers for $n \geq 2$, use the three-step approach above.

It is clear why this approach is called *divide-and-conquer*. We reduce the problem of multiplying $a \cdot b$ to some number of *simpler* problems of the same kind. A divide and conquer algorithm always consists of three parts: in the first part, we split the original problem into simpler problems of the same kind (our step (a)), in the second part we solve the simpler problems using the same method (our step (b)), and in the third part, we obtain the solution to the original problem from the solutions to the subproblems (our step (c)).

What is the connection of our recursive integer multiplication to the school method? It is really the same method. Figure 1.3 shows that the products $a_1 \cdot b_1$, $a_1 \cdot b_0$, $a_0 \cdot b_1$, and $a_0 \cdot b_0$ are also computed by the school method. Knowing that our recursive integer multiplication is just the school method in disguise tells us that the recursive algorithm uses a quadratic number of primitive operations. Let us also derive this from first principles. This will allow us to introduce recurrence relations, a powerful concept for the analysis of recursive algorithm.

Lemma 2. *Let $T(n)$ be the maximal number of primitive operations required by our recursive multiplication algorithm when applied to n-digit integers. Then*

$$T(n) \leq \begin{cases} 1 & \textit{if } n = 1, \\ 4 \cdot T(\lceil n/2 \rceil) + 3 \cdot 2 \cdot n & \textit{if } n \geq 2. \end{cases}$$

Proof. Multiplying two 1-digit numbers requires one primitive multiplication. This justifies the case $n = 1$. So assume $n \geq 2$. Splitting a and b into the four pieces

a_1, a_0, b_1, and b_0 requires no primitive operations[8]. Each piece has at most $\lceil n/2 \rceil$ digits and hence the four recursive multiplications require at most $4 \cdot T(\lceil n/2 \rceil)$ primitive operations. Finally, we need three additions to assemble the final result. Each addition involves two numbers of at most $2n$ digits and hence requires at most $2n$ primitive operations. This justifies the inequality for $n \geq 2$.

In Section 2.6 we will learn that such recurrences are easy to solve and yield the already conjectured quadratic execution time of the recursive algorithm.

Lemma 3. *Let $T(n)$ be the maximal number of primitive operations required by our recursive multiplication algorithm when applied to n-digit integers. Then $T(n) \leq 7n^2$ if n is a power of two and $T(n) \leq 28n^2$ for all n.*

Proof. We refer the reader to Section 1.8 for a proof.

1.5 Karatsuba Multiplication

In 1962 the Soviet mathematician Karatsuba [101] discovered a faster way of multiplying large integers. The running time of his algorithm grows like $n^{\log 3} \approx n^{1.58}$. The method is surprisingly simple. Karatsuba observed that a simple algebraic identity allows one multiplication to be eliminated in the divide-and-conquer implementation, i.e., one can multiply n-bit numbers using only *three* multiplications of integers half the size.

The details are as follows. Let a and b be our two n-digit integers which we want to multiply. Let $k = \lfloor n/2 \rfloor$. As above, we split a into two numbers a_1 and a_0; a_0 consists of the k least significant digits and a_1 consists of the $n-k$ most significant digits. We split b in the same way. Then

$$a = a_1 \cdot B^k + a_0 \quad \text{and} \quad b = b_1 \cdot B^k + b_0$$

and hence (the magic is in the second equality)

$$\begin{aligned} a \cdot b &= a_1 \cdot b_1 \cdot B^{2k} + (a_1 \cdot b_0 + a_0 \cdot b_1) \cdot B^k + a_0 \cdot b_0 \\ &= a_1 \cdot b_1 \cdot B^{2k} + ((a_1 + a_0) \cdot (b_1 + b_0) - (a_1 \cdot b_1 + a_0 \cdot b_0)) \cdot B^k + a_0 \cdot b_0 \end{aligned}$$

At first sight, we have only made things more complicated. A second look shows that the last formula can be evaluated with only three multiplications, namely, $a_1 \cdot b_1$, $a_1 \cdot b_0$, and $(a_1 + a_0) \cdot (b_1 + b_0)$. We also need six additions[9]. That is three more than in the recursive implementation of the school method. The key is that additions are cheap compared to multiplications and hence saving a multiplication more than outweighs three additional additions. We obtain the following algorithm for computing $a \cdot b$:

1. Split a and b into a_1, a_0, b_1, and b_0.

[8] It will require work, but it is work that we do not account for in our analysis.

[9] Actually five additions and one subtraction. We leave it to the reader to convince himself that subtractions are no harder than additions.

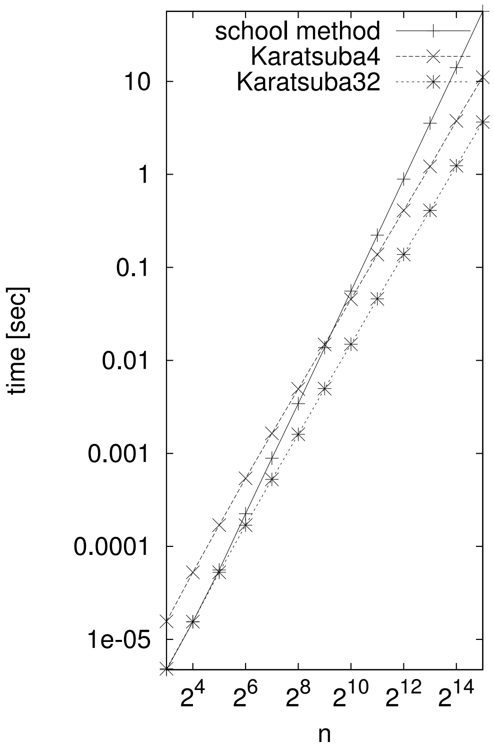


Fig. 1.4. The running times of implementations of the Karatsuba and the school method for integer multiplication. The running times for two versions of Karatsuba's method are shown: Karatsuba4 switches to the school method for integers with less than four digits and Karatsuba32 switches to the school method for integers with less than 32 digits. The slope of the lines for the Karatsuba variants is approximately 1.58.

2. Compute the three products $p_2 = a_1 \cdot b_1$, $p_0 = a_0 \cdot b_0$, and $p_1 = (a_1 + a_0) \cdot (b_1 + b_0)$.
3. Add the suitably aligned products to obtain $a \cdot b$, i.e., compute $a \cdot b$ according to the formula $a \cdot b = p_2 \cdot B^{2k} + (p_1 - (p_2 + p_0)) \cdot B^k + p_0$.

The numbers a_1, a_0, b_1, b_0, $a_1 + a_0$, and $b_1 + b_0$ are $\lceil n/2 \rceil + 1$-digit numbers and hence the multiplications in step (b) are simpler than the original multiplication if $\lceil n/2 \rceil + 1 < n$, i.e., $n \geq 4$. The complete algorithm is now as follows: to multiply 3-digit numbers, use the school method, and to multiply n-digit numbers for $n \geq 4$, use the three-step approach above.

Figure 1.4 shows the running times $T_K(n)$ and $T_S(n)$ of C++ implementations of the Karatsuba method and the school method for n-digit integers. The scale on both axes is logarithmic. We essentially see straight lines of different slope. The running time of the school method grows like n^2 and hence the slope is 2 in case of the school method. The slope is smaller in case of the Karatsuba method and this suggests that its running time grows like n^{β} with $\beta < 2$. In fact, the ratio[10] $T_K(n)/T_K(n/2)$ is close to three and this suggests that β is such that $2^{\beta} = 3$ or $\beta = \log 3 \approx 1.58$. Alternatively, you may determine the slope from Figure 1.4. We will prove below that $T_K(n)$ grows like $n^{\log 3}$. We say that the *Karatsuba method has better asymptotic behavior*. We also see that inputs have to be quite big until the superior asymptotic behavior of the Karatsuba method actually results in smaller running time. Observe that for $n = 2^8$, the school method is still faster, that for $n = 2^9$, the two methods have about the same running time, and that Karatsuba wins for $n = 2^{10}$. The lessons to remember are:

- Better asymptotic behavior ultimately wins.
- An asymptotically slower algorithm can be faster on small inputs.

In the next section we will learn how to improve the behavior of the Karatsuba method for small inputs. The resulting algorithm will always be at least as good as the school method. It is time to derive the asymptotics of the Karatsuba method.

Lemma 4. *Let $T_K(n)$ be the maximal number of primitive operations required by the Karatsuba algorithm when applied to n-digit integers. Then*

$$T_K(n) \le \begin{cases} 3n^2 + 2n & \text{if } n \le 3, \\ 3 \cdot T_K(\lceil n/2 \rceil + 1) + 6 \cdot 2 \cdot n & \text{if } n \ge 4. \end{cases}$$

Proof. Multiplying two n-bit numbers with the school method requires no more than $3n^2 + 2n$ primitive operations by Lemma 2. This justifies the first line. So assume $n \ge 4$. Splitting a and b into the four pieces a_1, a_0, b_1, and b_0 requires no primitive operations[11]. Each piece and the sums $a_0 + a_1$ and $b_0 + b_1$ have at most $\lceil n/2 \rceil + 1$ digits and hence the three recursive multiplications require at most $3 \cdot T_K(\lceil n/2 \rceil + 1)$ primitive operations. Finally, we need two additions to form $a_0 + a_1$ and $b_0 + b_1$ and four additions to assemble the final result. Each addition involves two numbers of at most $2n$ digits and hence requires at most $2n$ primitive operations. This justifies the inequality for $n \ge 4$.

In Section 2.6 we will learn general techniques for solving recurrences of this kind.

Theorem 3. *Let $T_K(n)$ be the maximal number of primitive operations required by the Karatsuba algorithm when applied to n-digit integers. Then $T_K(n) \le 99n^{\log 3} + 48 \cdot n + 48 \cdot \log n$ for all n.*

Proof. We refer the reader to Section 1.8 for a proof.

[10] $T_K(1024) = 0.0455$, $T_K(2048) = 0.1375$, and $T_K(4096) = 0.41$.

[11] It will require work, but it is work that we do not account for in our analysis.

1.6 Algorithm Engineering

Karatsuba integer multiplication is superior to the school method for large inputs. In our implementation the superiority only shows for integers with more than 1000 digits. However, a simple refinement improves the performance significantly. Since the school method is superior to Karatsuba for short integers, we should stop the recursion earlier and switch to the school method for numbers which have less than n_0 digits for some yet to be determined n_0. We call this approach the *refined Karatsuba method*. It is never worse than either the school method or the original Karatsuba algorithm.

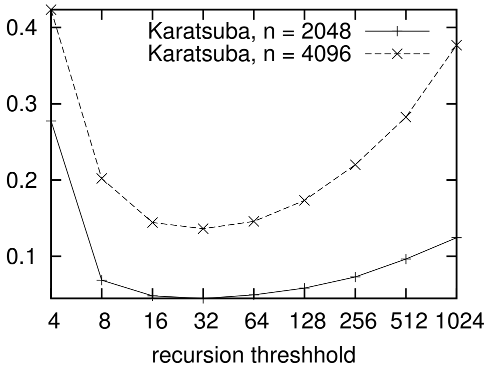


Fig. 1.5. The running time of the Karatsuba method as a function of the recursion threshold n_0. The times for multiplying 2048-digit and 4096-digit integers are shown. The minimum is at $n_0 = 32$.

What is a good choice for n_0? We will answer this question experimentally and analytically. Let us discuss the experimental approach first. We simply time the refined Karatsuba algorithm for different values of n_0 and then adopt the value giving the smallest running time. For our implementation the best results were obtained for $n_0 = 32$, see Figure 1.5. The asymptotic behavior of the refined Karatsuba method is shown in Figure 1.4. We see that the running time of the refined method still grows like $n^{\log 3}$, that the refined method is about three times faster than the basic Karatsuba method and hence the refinement is highly effective, and that the refined method is never slower than the school method.

Exercise 6. Derive a recurrence for the worst case number $T_R(n)$ of primitive operations performed by the refined Karatsuba method.

We can also approach the question analytically. If we use the school method to multiply n-digit numbers, we need $3n^2 + 2n$ primitive operations. If we use one Karatsuba step and then multiply the resulting numbers of length $\lceil n/2 \rceil + 1$ using the school method, we need about $3(3(n/2+1)^2 + 2(n/2+1)) + 12n$ primitive operations. The latter is smaller for $n \geq 28$ and hence a recursive step saves primitive operations as long as the number of digits is more than 28. You should not take this as an indication that an actual implementation should switch at integers of approximately 28 digits as the argument concentrates solely on primitive operations. You should take it as an argument, that it is wise to have a non-trivial recursion threshold n_0 and then determine the threshold experimentally.

Exercise 7. Throughout this chapter we assumed that both arguments of a multiplication are n-digit integers. What can you say about the complexity of multiplying n-digit and m-digit integers? (a) Show that the school method requires no more than $\alpha \cdot nm$ primitive operations for some constant α. (b) Assume $n \geq m$ and divide a into $\lceil n/m \rceil$ numbers of m digits each. Multiply each of the fragments with b using Karatsuba's method and combine the results. What is the running time of this approach?

1.7 The Programs

We give C++ programs for the school and the Karatsuba method. The programs were used for the timing experiments in this chapter. The programs were executed on a 2 GHz dual core Intel T7200 with 2 Gbyte of main memory and 4 MB of cache memory. The programs were compiled with GNU C++ version 3.3.5 using optimization level `-O2`.

A digit is simply an unsigned int and an integer is a vector of digits; here vector is the vector type of the standard template library. A declaration $\mathit{integer}\ a(n)$ declares an integer with n digits, $a.\mathit{size}()$ returns the size of a and $a[i]$ returns a reference to the i-th digit of a. Digits are numbered starting at zero. The global variable B stores the base. Functions $\mathit{fullAdder}$ and $\mathit{digitMult}$ implement the primitive operations on digits. We sometimes need to access digits beyond the size of an integer; the function $\mathit{getDigit}(a,i)$ returns $a[i]$ if i is a legal index for a and returns zero otherwise.

```
typedef unsigned int digit;
typedef vector<digit> integer;
unsigned int B = 10;                          // Base, 2 <= B <= 2^16

void fullAdder(digit a, digit b, digit c, digit& s, digit& carry)
{ unsigned int sum = a + b + c; carry = sum/B; s = sum - carry*B; }

void digitMult(digit a, digit b, digit& s, digit& carry)
{ unsigned int prod = a*b; carry = prod/B; s = prod - carry*B; }

digit getDigit(const integer& a, int i)
{ return ( i < a.size()? a[i] : 0 ); }
```

We want to run our programs on random integers: $\mathit{randDigit}$ is a simple random generator for digits and $\mathit{randInteger}$ fills its argument with random digits.

```
unsigned int X = 542351;

digit randDigit() { X = 443143*X + 6412431; return X % B ; }

void randInteger(integer& a)
{ int n = a.size(); for (int i = 0; i < n; i++) a[i] = randDigit(); }
```

We come to the school method of multiplication. We start with a routine that multiplies an integer a with a digit b and returns the result in $atimesb$. In each iteration, we compute d and c such that $c * B + d = a[i] * b$. We then add d, the c from the previous iteration, the $carry$ from the previous iteration, store the result in $atimesb[i]$, and remember the $carry$. The school method (function $mult$) multiplies a with each digit of b and then adds it at the appropriate position to the result (function $addAt$).

```
void mult(const integer& a, const digit& b, integer& atimesb)
{ int n = a.size(); assert(atimesb.size() == n+1);
  digit carry = 0, c, d, cprev = 0;

  for (int i = 0; i < n; i++)
    { digitMult(a[i],b,d,c);
      fullAdder(d, cprev, carry, atimesb[i], carry); cprev = c;
    }
  d = 0;
  fullAdder(d, cprev, carry, atimesb[n], carry);  assert(carry == 0);
}

void addAt(integer& p, const integer& atimesbj, int j)
{ // p has length n+m,
  digit carry = 0; int L = p.size();
  for (int i = j; i < L; i++)
    fullAdder(p[i], getDigit(atimesbj,i-j), carry, p[i], carry);
  assert(carry == 0);
}

integer mult(const integer& a, const integer& b)
{ int n = a.size(); int m = b.size();
  integer p(n + m,0);  integer atimesbj(n+1);
  for (int j = 0; j < m; j++)
    { mult(a, b[j], atimesbj); addAt(p, atimesbj, j); }
  return p;
}
```

For Karatsuba's method we also need methods for general addition and subtraction. The subtraction method may assume that the first argument is no smaller than the second. It computes its result in the first argument.

```
integer add(const integer& a, const integer& b)
{ int n = max(a.size(),b.size());
  integer s(n+1); digit carry = 0;
  for (int i = 0; i < n; i++)
      fullAdder(getDigit(a,i), getDigit(b,i), carry, s[i], carry);
  s[n] = carry;
  return s;
}

void sub(integer& a, const integer& b) // requires a >= b
{ digit carry = 0;

  for (int i = 0; i < a.size(); i++)
    if ( a[i] >= ( getDigit(b,i) + carry ))
```

```
      { a[i] = a[i] - getDigit(b,i) - carry; carry = 0; }
    else { a[i] = a[i] + B - getDigit(b,i) - carry; carry = 1;}
  assert(carry == 0);
}
```

The function *split* splits an integer into two integers of half the size.

```
void split(const integer& a,integer& a1,  integer& a0)
{ int n = a.size(); int k = n/2;
  for (int i = 0; i < k; i++) a0[i] = a[i];
  for (int i = 0; i < n - k; i++) a1[i] = a[k+ i];
}
```

Karatsuba works exactly as described in the text. If the inputs have less than *n0* digits, the school method is employed. Otherwise, the inputs are split into numbers of half the size and the products *p0*, *p1*, and *p2* are formed. Then *p0* and *p2* are written into the output vector, subtracted from *p1*, and finally the modified *p1* is added to the result.

```
integer Karatsuba(const integer& a, const integer& b, int n0)
{ int n = a.size(); int m = b.size(); assert(n == m); assert(n0 >= 4);
  integer p(2*n);

  if (n < n0) return mult(a,b);

  int k = n/2; integer a0(k), a1(n - k), b0(k), b1(n - k);

  split(a,a1,a0); split(b,b1,b0);

  integer p2 = Karatsuba(a1,b1,n0),
          p1 = Karatsuba(add(a1,a0),add(b1,b0),n0),
          p0 = Karatsuba(a0,b0,n0);

  for (int i = 0; i < 2*k; i++) p[i] = p0[i];
  for (int i = 2*k; i < n+m; i++) p[i] = p2[i - 2*k];

  sub(p1,p0); sub(p1,p2); addAt(p,p1,k);

  return p;
}
```

The following program generates the data for Figure 1.4.

```
inline double cpuTime() { return double(clock())/CLOCKS_PER_SEC; }

int main(){

for (int n = 8; n <= 131072; n *= 2)
{ integer a(n),  b(n); randInteger(a); randInteger(b);

  double T = cpuTime();  int k = 0;
  while (cpuTime() - T < 1) {  mult(a,b); k++; }
  cout << "\n" << n << " school = " << (cpuTime() - T)/k;
  T = cpuTime(); k = 0;
  while (cpuTime() - T < 1) {  Karatsuba(a,b,4); k++; }
  cout << " Karatsuba4 = " << (cpuTime() - T) /k; cout.flush();

  T = cpuTime(); k = 0;
  while (cpuTime() - T < 1) {  Karatsuba(a,b,32); k++; }
  cout << " Karatsuba32 = " << (cpuTime() - T) /k; cout.flush();
}
return 0;
}
```

1.8 The Proofs of Lemma 3 and Theorem 3

To make this Chapter self-contained, we include proofs of Lemma 3 and Theorem 3. We start with the analysis of the recursive version of the school method. Recall that $T(n)$, the maximal number of primitive operations required by our recursive multiplication algorithm when applied to n-digit integers, satisfisfies

$$T(n) \le \begin{cases} 1 & \text{if } n = 1, \\ 4 \cdot T(\lceil n/2 \rceil) + 3 \cdot 2 \cdot n & \text{if } n \ge 2. \end{cases}$$

We use induction on n to show $T(n) \le 7n^2 - 6n$ for n being a power of two. For $n = 1$, we have $T(1) \le 1 = 7n^2 - 6n$. For $n > 1$, we have

$$T(n) \le 4T(n/2) + 6n \le 4(7(n/2)^2 - 6n/2) + 6n = 7n^2 - 6n\ ,$$

where the second inequality follows from the induction hypothesis. For general n, we observe that multiplying n-digit integers is certainly no more costly than multiplying $2^{\lceil \log n \rceil}$-digit integers and hence $T(n) \le T(2^{\lceil \log n \rceil})$. Since $2^{\lceil \log n \rceil} \le 2n$, we conclude $T(n) \le 28n^2$ for all n.

Exercise 8. Prove a bound on the recurrence $T(1) \le 1$ and $T(n) \le 4T(n/2) + 9n$ for n a power of two.

How did we know that "$7n^2 - 6n$" is the bound to prove? There is no magic here. For $n = 2^k$ repeated substitution yields:

$$\begin{aligned} T(2^k) &\le 4 \cdot T(2^{k-1}) + 6 \cdot 2^k \le 4^2 T(2^{k-2}) + 6 \cdot (4^1 \cdot 2^{k-1} + 2^k) \\ &\le 4^3 T(2^{k-3}) + 6 \cdot (4^2 \cdot 2^{k-2} + 4^1 \cdot 2^{k-1} + 2^k) \le \ldots \\ &\le 4^k T(1) + 6 \sum_{0 \le i \le k-1} 4^i 2^{k-i} \le 4^k + 6 \cdot 2^k \sum_{0 \le i \le k-1} 2^i \\ &\le 4^k + 6 \cdot 2^k (2^k - 1) = n^2 + 6n(n-1) = 7n^2 - 6n\ . \end{aligned}$$

We turn to the proof of Theorem 3. Recall that T_K satisfies the recurrence

$$T_K(n) \le \begin{cases} 3n^2 + 2n & \text{if } n \le 3, \\ 3 \cdot T_K(\lceil n/2 \rceil + 1) + 12n & \text{if } n \ge 4. \end{cases}$$

The recurrence for the school method has the nice property that for n being a power of two, the arguments of T on the right-hand side were again powers of two. This is not true for T_K. However, if $n = 2^k + 2$ and $k \geq 1$ then $\lceil n/2 \rceil + 1 = 2^{k-1} + 2$ and hence we should now use numbers of the form $n = 2^k + 2$, $k \geq 0$, as the basis of the inductive argument. We show

$$T_K(2^k + 2) \leq 33 \cdot 3^k + 12 \cdot (2^{k+1} + 2k - 2)$$

for $k \geq 0$. For $k = 0$, we have

$$T_K(2^0 + 2) = T_K(3) \leq 3 \cdot 3^2 + 2 \cdot 3 = 33 = 33 \cdot 2^0 + 12 \cdot (2^1 + 2 \cdot 0 - 2) \; .$$

For $k \geq 1$, we have

$$\begin{aligned} T_K(2^k + 2) &\leq 3T_K(2^{k-1} + 2) + 12 \cdot (2^k + 2) \\ &\leq 3 \cdot (33 \cdot 3^{k-1} + 12 \cdot (2^k + 2(k-1) - 2) + 12 \cdot (2^k + 2) \\ &= 33 \cdot 3^k + 12 \cdot (2^{k+1} + 2k - 2) \; . \end{aligned}$$

Again, there is no magic in coming up with the right induction hypothesis. It is obtained by repeated substitution. Namely,

$$\begin{aligned} T_K(2^k + 2) &\leq 3T_K(2^{k-1} + 2) + 12 \cdot (2^k + 2) \\ &\leq 3^k T_K(2^0 + 2) + 12 \cdot (2^k + 2 + 2^{k-1} + 2 + \ldots + 2^1 + 2) \\ &\leq 33 \cdot 3^k + 12 \cdot (2^{k+1} - 2 + 2k) \; . \end{aligned}$$

It remains to extend the bound to all n. Let k be the minimal integer with $n \leq 2^k + 2$. Then $k \leq 1 + \log n$. Also, multiplying n-digit numbers is no more costly than multiplying $(2^k + 2)$-digit numbers and hence

$$\begin{aligned} T_K(n) &\leq 33 \cdot 3^k + 12 \cdot (2^{k+1} - 2 + 2k) \\ &\leq 99 \cdot 3^{\log n} + 48 \cdot (2^{\log n} - 2 + 2(1 + \log n)) \\ &\leq 99 \cdot n^{\log 3} + 48 \cdot n + 48 \cdot \log n \; , \end{aligned}$$

where the equality $3^{\log n} = 2^{(\log 3) \cdot (\log n)} = n^{\log 3}$ is used.

Exercise 9. Solve the recurrence

$$T_R(n) \leq \begin{cases} 3n^2 + 2n & \text{if } n < 32, \\ 3 \cdot T_R(\lceil n/2 \rceil + 1) + 12n & \text{if } n \geq 4. \end{cases}$$

1.9 Implementation Notes

The programs given in Section 1.7 are not optimized. The base of the number system should be chosen as a power of two so that sums and carries can be extracted by bit operations. Also, the size of a digit should agree with the word size of the machine and a bit more work should be invested in implementing primitive operations on digits.

C++: GMP [74] and LEDA [115] offer high-precision integer, rational, and floating point arithmetic. Highly optimized implementations of Karatsuba's method are used for multiplication.

Java: `Java.math` implements arbitrary precision integers and floating point numbers. ⟹ [font fuer java.math]

1.10 Historical Notes and Further Findings

Is the Karatsuba method the fastest known method for integer multiplication? No, much faster methods are known. Karatsuba's method splits integer into two parts and requires three multiplications of integers of half the length. The natural extension is to split into k parts of length n/k each. If the recursive step requires ℓ multiplications of numbers of length n/k, the running time of resulting algorithm grows like $n^{\log_k \ell}$. In this way, Toom [185] and Cook [44] reduced the running time to[12] $\mathcal{O}\big(n^{1+\epsilon}\big)$ for arbitrary positive ϵ. The asymptotically most efficient algorithms are the work of Schönhage and Strassen [161] and Schönhage [160]. The former multiplies n-bit integers with $\mathcal{O}(n \log n \operatorname{loglog} n)$ bit operations and it can be implemented to run in this time bound on a Turing machine. The latter runs in linear time $\mathcal{O}(n)$ and requires the machine model discussed in Section 2.2. In this model, integers with $\log n$ bits can be multiplied in constant time.

[12] $\mathcal{O}(\cdot)$-notation is defined in Section 2.1.

2

Introduction

[Stonehenge.png verwenden ?] ⟸

When you want to become a sculptor, you will have to learn some basic techniques: Where to get the right stones, how to move them, how to handle the chisel, how to erect scaffolding, ... Knowing these techniques will not make you a famous artist, but even if you are a really exceptional talent, it will be very difficult to develop into a successful artist without knowing them. It is not necessary to master all basic techniques, before sculpting the first piece. But you always have to be willing to go back to improve your basic techniques.

This introductory chapter plays a similar role for this book. We introduce basic concepts that make it simpler to discuss and analyze algorithms in the subsequent chapters. There is no need for you to read this chapter from beginning to end before you proceed to later chapters. On first reading, we recommend to read carefully till the end of Section 2.3 and to skim through the remaining sections. We begin in Section 2.1 by introducing notation and terminology that allows us to argue about the complexity of algorithms in a concise way. We then introduce a simple machine model in Section 2.2 that allows us to abstract from the highly variable complications introduced by real hardware. The model is concrete enough to have predictive value and abstract enough to allow elegant arguments. Section 2.3 then introduces a high level pseudocode notation for algorithms that is much more convenient for expressing algorithms than the machine code of our abstract machine. Pseudocode is also more convenient than actual programming languages since we can use high level concepts borrowed from mathematics without having to worry about how exactly they can be compiled to run on actual hardware. We frequently annotate programs to make algorithms more readable and easier to prove correct. This is the content of Section 2.4. Section 2.5 gives a first comprehensive example: binary search in a sorted array. In Section 2.6 we introduce mathematical techniques for analyzing the complexity of programs, in particular, for analyzing nested loops and recursive procedure calls. Additional analysis techniques are needed for average case analysis which are covered in Section 2.7. Randomized algorithms, discussed in Section 2.8

use coin tosses in their execution. Section 2.9 is devoted to graphs, a concept that will play an important role throughout the book. In Section 2.10 we discuss the question when an algorithm should be called efficient and introduce complexity classes $\mathbf{P}$ and $\mathbf{NP}$. Finally, as in every chapter of this book, there are sections on implementation notes (Section 2.11) and on historical notes and further findings (Section 2.12).

2.1 Asymptotic Notation

The main purpose of algorithm analysis is to give performance guarantees, e.g, bounds on running time, that are at the same time accurate, concise, general, and easy to understand. It is difficult to meet all these criteria simultaneously. For example, the most accurate way to characterize the running time T of an algorithm is to view T as a mapping from the set I of all inputs to the set of nonnegative numbers $\mathbb{R}_+$. For any problem instance i, $T(i)$ is the running time on i. This level of detail is so overwhelming that we could not possibly derive a theory on it. A useful theory needs a more global view on the performance of an algorithm.

We group the set of all inputs into classes of "similar" inputs and summarize the performance on all instances in the same class into a single number. The most useful grouping is by *size*. Usually, there is a natural way to assign a size to each problem instance. The size of an integer is the number of digits in its representation and the size of a set is the number of elements in the set. The size of an instance is always a natural number. Sometimes, we will use more than one parameter to measure the size of an instance; for example, it is customary to measure the size of a graph by its number of nodes and by its number of edges. We ignore this complication for now. We use $\mathrm{size}(i)$ to denote the size of instance i and I_n to denote the instances of size n for $n \in \mathbb{N}$. For the inputs of size n, we are interested in the maximum, minimum, and average execution time.[1]

$$\begin{array}{ll}\textbf{worst case:} & T(n) = \max\{T(i) : i \in I_n\} \\ \textbf{best case:} & T(n) = \min\{T(i) : i \in I_n\} \\ \textbf{average case:} & T(n) = \frac{1}{|I_n|}\sum_{i \in I_n} T(i)\end{array}$$

We are most interested in the worst case execution time since it gives us the strongest performance guarantee. The comparison of the best case and the worst case tells us how much the execution time varies for different inputs in the same class. If the discrepancy is big, the average case may give more insight into the true performance of the algorithm. Section 2.7 gives an example.

We are going to make one more step of data reduction. We will concentrate on *growth rate* or *asymptotic analysis*. Functions $f(n)$ and $g(n)$ have the *same growth rate* if there are positive constants c and d such that $c \leq f(n)/g(n) \leq d$ for all sufficiently large n and $f(n)$ *grows faster* than $g(n)$ if for all positive constants c, we have $f(n) \geq c \cdot g(n)$ for all sufficiently large n. For example, the functions n^2,

[1] We will make sure that $\{T(i) : i \in I_n\}$ always has a proper minimum and maximum, and that I_n is finite when we consider averages.

n^2+7n, $5n^2-7n$ and $n^2/10+10^6n$ all have the same growth rate. Also, they grow faster than $n^{3/2}$ which in turn grows faster than $n\log n$. Growth rate talks about the behavior for large n. The word "asymptotic" in asymptotic analysis also stresses the fact that we are interested in the behavior for large n.

Why are we only interested in growth rates and the behavior for large n? We are interested in the behavior for large n, since the whole purpose of designing efficient algorithms is to be able to solve large instances. For large n, an algorithm whose running time has smaller growth rate than the running time of another algorithm will be superior. Also, our machine model is an abstraction of real machines and hence can predict actual running time only up to a constant factor, and this suggests to make no difference between algorithms whose running time has the same growth rate. A pleasing side effect of concentrating on growth rate is that we can characterize the running times of algorithms by simple functions. However, in the sections on implementation we will frequently take a closer look and go beyond asymptotic analysis. Also, when using one of the algorithms described in this book, you should always ask yourself whether the asymptotic view is justified.

The following definitions allow us to argue precisely about *asymptotic behavior*. Let $f(n)$ and $g(n)$ denote functions that map nonnegative integers to nonnegative real numbers.

$$\mathcal{O}(f(n)) = \{g(n) : \exists c>0 : \exists n_0 \in \mathbb{N}_+ : \forall n \geq n_0 : g(n) \leq c\cdot f(n)\} \tag{2.1}$$

$$\Omega(f(n)) = \{g(n) : \exists c>0 : \exists n_0 \in \mathbb{N}_+ : \forall n \geq n_0 : g(n) \geq c\cdot f(n)\} \tag{2.2}$$

$$\Theta(f(n)) = \mathcal{O}(f(n)) \cap \Omega(f(n)) \tag{2.3}$$

$$o(f(n)) = \{g(n) : \forall c>0 : \exists n_0 \in \mathbb{N}_+ : \forall n \geq n_0 : g(n) \leq c\cdot f(n)\} \tag{2.4}$$

$$\omega(f(n)) = \{g(n) : \forall c>0 : \exists n_0 \in \mathbb{N}_+ : \forall n \geq n_0 : g(n) \geq c\cdot f(n)\} \tag{2.5}$$

The left-hand sides should be read as "big O of f", "big Omega of f", "Theta of f", "little o of f", and "little omega of f", respectively.

Let us see some examples. $\mathcal{O}(n^2)$ is the set of all functions that grow at most quadratically, $\mathrm{o}(n^2)$ is the set of functions that grow less than quadratically, and $\mathrm{o}(1)$ is the set of functions that go to zero as n goes to infinity. Here 1 stands for the function $n \mapsto 1$ which is one everywhere and hence $f \in \mathrm{o}(1)$ if $f(n) \leq c\cdot 1$ for any positive c and sufficiently large n, i.e., $f(n)$ goes to zero as n goes to infinity. Generally, $\mathcal{O}(f(n))$ is the set of all functions that "grow no faster than" $f(n)$. Similarly, $\Omega(f(n))$ is the set of all functions that "grow at least as fast as" $f(n)$. For example, the Karatsuba algorithm for integer multiplication has worst case running time in $\mathcal{O}(n^{1.58})$ whereas the school algorithm has worst case running time in $\Omega(n^2)$ so that we can say that the Karatsuba algorithm is asymptotically faster than the school algorithm. The "little-o" notation $o(f(n))$ denotes the set of all functions that "grow strictly more slowly than" $f(n)$. Its twin $\omega(f(n))$ is rarely used and only shown for completeness.

The growth rate of most algorithms discussed in this book is either a polynomial or a logarithmic function or the product of a polynomial and a logarithmic function. We use polynomials to introduce our readers into basic manipulations of asymptotic notation.

Lemma 5. *Let* $p(n)=\sum_{i=0}^{k}a_i n^i$ *denote any polynomial and assume* $a_k>0$. *Then* $p(n)\in\Theta\big(n^k\big)$.

Proof. It suffices to show $p(n)\in\mathcal{O}\big(n^k\big)$ and $p(n)\in\Omega\big(n^k\big)$. First observe that for $n>0$,

$$p(n)\le\sum_{i=0}^{k}|a_i|n^i\le n^k\sum_{i=0}^{k}|a_i|\ ,$$

$\Longrightarrow$ and hence $p(n)\le(\sum_{i=0}^{k}|a_i|)n^k$ for all positive n. Thus[mit oder ohne komma?] $p(n)\in\mathcal{O}\big(n^k\big)$.

Let $A=\sum_{i=0}^{k-1}|a_i|$. For positive n we have

$$p(n)\ge a_k n^k-An^{k-1}=\frac{a_k}{2}n^k+n^{k-1}(\frac{a_k}{2}n-A)$$

and hence $p(n)\ge(a_k/2)n^k$ for $n>2A/a_k$. We chose $c=a_k/2$ and $n_0=2A/a_k$ in the definition of $\Omega\big(n^k\big)$, and obtain $p(n)\in\Omega\big(n^k\big)$.

Exercise 10. Right or wrong? (a) $n^2+10^6n\in\mathcal{O}\big(n^2\big)$, (b) $n\log n\in\mathcal{O}(n)$, (c) $n\log n\in\Omega(n)$, (d) $\log n\in\mathrm{o}(n)$.

Asymptotic notation is used a lot in algorithm analysis and it is convenient to stretch mathematical notation a bit in order to allow treating sets of functions (such as $\mathcal{O}\big(n^2\big)$) similarly to ordinary functions. In particular, we will always write $h=\mathcal{O}(f)$ instead of $h\in\mathcal{O}(f)$ and $\mathcal{O}(h)=\mathcal{O}(f)$ instead of $\mathcal{O}(h)\subseteq\mathcal{O}(f)$. For example,

$$3n^2+7n=\mathcal{O}\big(n^2\big)=\mathcal{O}\big(n^3\big)\ .$$

Be warned that sequences of equalities involving $\mathcal{O}$-notation should only be read from left to right.

If h is a function, F and G are sets of functions and '$\circ$' is an operator like $+$, $\cdot$, $/$,... then $F\circ G$ is a shorthand for $\{f\circ g : f\in F, g\in G\}$ and $h\circ F$ stands for $\{h\}\circ F$. So $f(n)+o(f(n))$ denotes the set of all functions $f(n)+g(n)$ where $g(n)$ grows strictly slower than $f(n)$, i.e., the ratio $(f(n)+g(n))/f(n)$ goes to one as n goes to infinity. Equivalently, we can write $(1+o(1))f(n)$. We use this notation whenever we care about the constant in the leading term but want to ignore *lower order terms*.

Lemma 6. *The following rules hold for* $\mathcal{O}$*-notation:*

$$\begin{aligned}
cf(n)&=\Theta(f(n))\ \textit{for any positive constant } c && (2.6)\\
f(n)+g(n)&=\Omega(f(n)) && (2.7)\\
f(n)+g(n)&=\mathcal{O}(f(n))\ \textit{if } g(n)=\mathcal{O}(f(n)) && (2.8)\\
\mathcal{O}(f(n))\cdot\mathcal{O}(g(n))&=\mathcal{O}(f(n)\cdot g(n)) && (2.9)
\end{aligned}$$

Exercise 11. Prove Lemma 6.

Exercise 12. Sharpen Lemma 5 and show $p(n)=a_k n^k+o(n^k)$.

2.2 Machine Model

In 1945 John von Neumann introduced a computer architecture [142] which is simple and yet powerful. The limited hardware technology of the time forced him to come up with an elegant design concentrating on the essentials; otherwise, realization would have been impossible. Hardware technology has developed tremendously since 1945. However, the programming model resulting from von Neumann's design is so elegant and powerful, that it is still the basis for most of modern programming. Usually, programs written with von Neumann's model in mind also work well on the vastly more complex hardware of today's machines.

Fig. 2.1. John von Neumann born Dec. 28, 1903 in Budapest, died Feb. 8, 1957, Washington DC.

The variant of von Neumann's model used in algorithmic analysis is called the *RAM (random access machine)* model. It was introduced by Sheperdson and Sturgis [168]. It is a *sequential* machine with uniform memory, i.e., there is a single processing unit and all memory accesses take the same amount of time. The memory or *s*tore consists of infinitely many cells $S[0]$, $S[1]$, $S[2]$, $\ldots$; at any point in time, only a finite number of them will be in use.

The memory cells store "small" integers. In our discussion of integer arithmetic in Chapter 1, we assumed that small means one digit. It is more reasonable and convenient to assume that the interpretation of "small" depends on the input size. Our default assumption is that integers bounded by a polynomial in the size of the data being processed can be stored in a single cell. Such integers can be represented with a number of bits that is logarithmic in the size of the input. The assumption is reasonable because we could always spread out the content of a single cell over logarithmically many cells for a logarithmic overhead in time and space and obtain constant size cells. The assumption is convenient because we want to be able to store array indices in a single cell. The assumption is necessary, since allowing cells to store arbitrary numbers would lead to absurdly over-optimistic algorithms. For example, by repeated squaring, we could generate a number with 2^n bits in n steps. Namely, if we start with the number $2 = 2^1$, squaring it once gives $4 = 2^2 = 2^{2^1}$, squaring it twice gives $16 = 2^4 = 2^{2^2}$, and squaring it n times gives 2^{2^n}. Our model supports a limited form of parallelism. We can perform simple operations on a logarithmic number of bits in constant time.

In addition to the main memory, there is a small number of *registers* $R_1, \ldots, R_k$. Our RAM can execute the following *machine instructions*.

$R_i := S[R_j]$ *loads* the content of the memory cell indexed by the content of R_j into register R_i.

$S[R_j] := R_i$ *stores* register R_i into the memory cell indexed by the content of R_j.

$R_i := R_j \odot R_\ell$ is a binary register operation where '$\odot$' is a placeholder for a variety of operations. *Arithmetic* operations are the the usual $+$, $-$, and $*$ but also the bit-wise operations `|` (or), `&` (and), >> (shift right), << (shift left), and $\oplus$ (exclusive or). Operations **div** and **mod** stand for integer division and remainder respectively. *Comparison* operations $\leq$, $<$, $>$, $\geq$ yield $true$ (= 1) or *false* (= 0). *Logical* operations $\wedge$ and $\vee$ manipulate the *truth values* 0 and 1. We may also assume that there are operations which interpret the bits stored in a register as a floating point number, i.e., a finite precision approximation of a real number.

$R_i := \odot R_j$ is a *unary* operation using the operators $-$, $\neg$ (logical not), or ~ (bitwise not).

$R_i := C$ assigns a *constant* value to R_i.

`JZ` j, R_i continues execution at memory address j if register i is zero.

`J` j continues execution at memory address j.

Each instruction takes one time step to execute. The total execution time of a program is the number of instructions executed. A program is a list of instructions numbered starting at one. The addresses in jump-instructions refer to this numbering. The input for a computation is stored in memory cells $S[1]$ to $S[R_1]$.

It is important to remember that the RAM model is an abstraction. One should not confuse it with physically existing machines. In particular, real machines have finite memory and a fixed number of bits per register (e.g., 32 or 64). In contrast, word size and memory of a RAM scales with input size. This can be viewed as an abstraction of historical development. Microprocessors subsequently had 4, 8, 16, 32, and now often 64 bit words. Words with 64 bits can index a memory of size 2^{64}. Thus at current prices, memory size is limited by cost and not by physical limitations. Observe, that this statement was also true when 32-bit words were introduced.

Our complexity model is also a gross oversimplification: Modern processors attempt to execute many instructions in parallel. How well they succeed depends on factors like data dependencies between subsequent operations. As a consequence, an operation does not have a fixed cost. This effect is particularly pronounced for memory accesses. The worst case time for a memory access from main memory can be hundreds of times higher than the best case time. The reason is that modern processors attempt to keep frequently used data in *caches* — small, fast memories close to the processors. How well caches work depends a lot on their architecture, the program, and the particular input.

We could attempt to introduce a very accurate cost model but this would miss the point. We would end up with a complex model that is difficult to handle. Even a successful complexity analysis would be a monstrous formula depending on many parameters that change with every new processor generation. Although such a formula would contain detailed information, the very complexity of the formula would make it useless. We therefore go to the other extreme and eliminate all model parameters by assuming that each instruction takes exactly one unit of time. The result is that constant factors in our model are quite meaningless — one more reason to stick to asymptotic analysis most of the time. We compensate this drawback by implementation notes in which we discuss implementation choices and tradeoffs.

External Memory: The biggest difference between a RAM and real machines is the memory: a uniform memory in a RAM and a complex memory hierarchy in real machines. In Sections 5.7, 6.3 and 7.6 we will discuss algorithms which are specifically designed for huge data sets which have to be stored on slow memory, such a disks. We will use the so-called *external memory model* to study these algorithms.

The external memory model is like the RAM model except that the fast memory S is limited in size to M words. Additionally, there is an external memory with unlimited size. There are special *I/O operations* that transfer B consecutive words between slow and fast memory. For example, the external memory could be a hard disk, M would then be the main memory size and B would be a block size that is a good compromise between low latency and high bandwidth. On current technology, $M = 1$ GByte and $B = 1$ MByte are realistic values. One I/O step would then be around 10ms which is 10^7 clock cycles of a 1GHz machine. With another setting of the parameters M and B, we could model the smaller access time difference between a hardware cache and main memory.

Parallel Processing: On modern machines, we are confronted with many forms of parallel processing. Many processors have 128–512 bit wide *SIMD* registers that allow the parallel execution of a **S**ingle **i**nstruction on **m**ultiple **d**ata objects. *Simultaneous multi-threading* allows processors to better utilize their resources by running multiple threads of activity on a single processor core. Even mobile devices often have multiple processor cores that can independently execute a program and most servers have several such *multicore* processors accessing the same *shared memory*. Co-processors, in particular for graphics processing, have even more parallelism on a single chip. High performance computers consist of multiple server-type systems interconnected by a fast, dedicated network. Finally, more loosely connected computers of all types interact through various kind of networks (internet, radio networks,...) in *distributed systems* that may consist of millions of nodes. As you can imagine, no single simple model can be used to describe parallel programs on these many levels of parallelism. We will therefore restrict ourselves to occasional informal arguments why a certain sequential algorithm may be more or less easy to adapt to parallel processing. For example, the algorithms for high precision arithmetics in Chapter 1 could make use of SIMD-instructions.

2.3 Pseudocode

Our RAM model is an abstraction and simplification of the machine programs executed on microprocessors. The purpose of the model is to have a precise definition of running time. However, the model is much too low level for formulating complex algorithms. Our programs would become too long and too hard to read. Instead we formulate our algorithms in *pseudocode* that is an abstraction and simplification of imperative programming languages like C, C++, Java, Pascal, etc. , combined with a liberal use of mathematical notation. We now describe the conventions used in this book and derive a timing model for pseudocode programs. The timing model is quite simple: *basic pseudocode instructions take constant time and procedure and function calls take constant time plus the time to execute their body*. We justify the timing model by outlining how pseudocode can be translated into equivalent RAM-code. We do this only to the extent necessary to understand the timing model. There is no need to worry about compiler optimization techniques since constant factors are outside our theory. The reader may decide to skip the paragraphs describing the translation and adopt the timing model as an axiom. The syntax of our pseudocode is akin to Pascal [97] because we find this notation typographically nicer for a book than the more widely known syntax of C and its descendents C++ and Java.

A *variable declaration* "$v = x\ : T$" introduces a variable v of type T and initializes it with value x. For example, "$answer = 42\ : \mathbb{N}$" introduces a variable $answer$ assuming integer values and initializes it to the value 42. When the type of a variable is clear from the context, we sometimes omit it from the declaration. A type is either a basic type (e.g., integer, boolean value, or pointer) or a composite type. We have predefined composite types such as arrays and application specific classes (see below). When the type of a variable is irrelevant for the discussion, we use the unspecified type $Element$ as a placeholder for an arbitrary type. We take the liberty of extending numeric types by values $-\infty$ and ∞, whenever this is convenient. Similarly, we sometimes extend types by an undefined value (denoted by the symbol $\perp$) which we assume to be distinguishable from any "proper" element of T. In particular, for pointer types it is useful to have an undefined value. The values of the pointer type "**Pointer to** T" are handles of objects of type T. In the RAM model, this is the index of the first cell in a region of storage holding an object of type T.

A declaration "$a : Array\ [i..j]$ **of** T" introduces an *array* a consisting of $j-i+1$ *elements* of type T stored in $a[i]$, $a[i+1]$, $\ldots$, $a[j]$. Arrays are implemented as contiguous pieces of memory. To find element $a[k]$, it suffices to know the starting address of a and the size of an object of type T. For example, if register R_a stores the starting address of array $a[0..k]$ and elements have unit size, the instruction sequence "$R_1{:=}R_a{+}42; R_2{:=}S[R_1]$" loads $a[42]$ into register R_2. The size of an array is fixed at the time of declaration; such arrays are also called *static*. In Section 3.2 we show how to implement *unbounded arrays* that can grow and shrink during execution.

A declaration "c : **Class** $age : \mathbb{N}$, $income : \mathbb{N}$ **end**" introduces a variable c whose values are pairs of integers. The components of c are denoted $c.age$ and $c.income$. For a variable c, **addressof** c returns the address of c. We also say, it returns a handle to c. If p is an appropriate pointer type, $p :=$ **addressof** c stores a handle to c in p and $*p$ gives us back c. The fields of c can then also be accessed through $p \rightarrow age$ and $p \rightarrow income$. Alternatively, one may write (but nobody ever does) $(*p).age$ and $(*p).income$.

Arrays and objects referenced by pointers can be allocated and deallocated by the commands **allocate** and **dispose**. For example, $p :=$ **allocate** $Array\ [1..n]$ **of** T allocates an array of n objects of type T, i.e., allocates a contiguous chunk of memory of size n times the size of an object of type T, and assigns a handle of this chunk (= starting address of the chunk) to p. Instruction **dispose** p frees this memory and makes it available for reuse. With **allocate** and **dispose** we cut our memory array S into disjoint pieces that can be referred to separately. The functions can be implemented to run in constant time. The most simple implementations is as follows. We keep track of the used portion of S, say *free* contains the index of the first free cell of S. A call of **allocate** reserves a chunk of memory starting at *free* and increases *free* by the size of the allocated chunk. A call of **dispose** does nothing. This implementation is time-efficient, but not space efficient. Any call of **allocate** or **dispose** takes constant time. However, the total space consumption is the total space ever allocated and not the maximal space simultaneously used, i.e., allocated but not yet freed, at any one time. It is not known whether an arbitrary sequence of **allocate** and **dispose** operations can be realized space-efficiently and with constant time per operation. However, for all algorithms presented in this book, **allocate** and **dispose** can be realized in a time and space efficient way. We will ask the reader to design efficient schemes in the exercises.

We borrow some composite data structures from mathematics, in particular, we will use tuples, sequences, and sets. *Pairs*, *Triples*, and, more generally, *Tuples* are written in round brackets, e.g., $(3, 1)$, $(3, 1, 4)$ or $(3, 1, 4, 1, 5)$. Since tuples only contain a constant number of elements, operations on them can be broken into operations on their constituents in an obvious way. *Sequences* store elements in a specified order, e.g., "$s = \langle 3, 1, 4, 1\rangle$: Sequence **of** $\mathbb{Z}$" declares a sequence s of integers and initializes it to contain the numbers 3, 1, 4, and 1 in this exact order. Sequences are a natural abstraction for many data structures like files, strings, lists, stacks, and queues. In Chapter 3 we will study many ways to represent sequences. In later chapters, we will make extensive use of sequences as a mathematical abstraction with little further reference to implementation details. The empty sequence is written as $\langle\rangle$.

Sets play an important role in mathematical arguments and we will also use them in our pseudocode. In particular, you will see declarations like "$M = \{3, 1, 4\}$: *Set* **of** $\mathbb{N}$" that are analogous to declarations of arrays or sequences. Sets are usually implemented as sequences.

Having discussed variables and their declaration, we come to statements. The simplest statement is an assignment $x := E$ where x is a variable and E is an expression. An assignment is easily transformed into a constant number of RAM instructions. For example, the statement $a := a + bc$ is translated into "$R_1 := R_b * R_c$; $R_a := R_a + R_1$" where R_a, R_b, and R_c stand for the registers storing a, b, and c respectively. From C we borrow the shorthands $++$ and $--$ for incrementing and decrementing variables. We also use parallel assignment to several variables. For example, if a and b are variables of the same type, "$(a, b) := (b, a)$" swaps the contents of a and b.

The conditional statement "**if** C **then** I **else** J", where C is a boolean expression and I and J are statements, translates into the instruction sequence

$$eval(C);\ \texttt{JZ}\ sElse\ R_c;\ trans(I);\ \texttt{J}\ sEnd;\ trans(J)$$

where $eval(C)$ is a sequence of instructions evaluating the expression C and storing its result in register R_c, $trans(I)$ is a sequence of instructions implementing statement I, $trans(J)$ implements J, $sElse$ is the address of the first instruction in

$trans(J)$, and $sEnd$ is the address of the first instruction after $trans(J)$. The sequence above first evaluates C. If C evaluates to false (= 0), the program jumps to the first instruction of the translation of J. If C evaluates to true (= 1), the program continues with the translation of I and then jumps to the instruction after the translation of J. The statement "**if** C **then** I" is a shorthand for "**if** C **then** I **else** ;", i.e., an if-then-else with an empty else part.

Our write-up of programs is intended for humans and uses less strict syntax than programming languages. In particular, we usually group statements by indentation and in this way avoid the the proliferation of brackets observed in programming languages like C that are designed as a compromise of readability for humans and computers. We use brackets only if the write-up would be ambiguous otherwise. For the same reason, a line break can replace a semicolon for separating statements.

The loop "**repeat** I **until** C" translates into $trans(I)$; $eval(C)$; `JZ` sI R_c where sI is the address of the first instruction in $trans(I)$. We will also use many other types of loops that can be viewed as shorthands for repeat-loops. In the following list, the shorthand on the left expands into the statements on the right.

while C **do** I	**if** C **then repeat** I **until** $\neg C$
for $i := a$ **to** b **do** I	$i := a$; **while** $i \leq b$ **do** I; i++
foreach $e \in s$ **do** I	**for** $i := 1$ **to** $\lvert s \rvert$ **do** $e := s[i]$; I

Many low level optimizations are possible when translating loops into RAM code. They are of no concern for us. For us, it is only important that the execution time of a loop can be bounded by summing the execution times of each of its iterations including the time needed for evaluating conditions.

A subroutine with name *foo* is declared in the form "**Procedure** $foo(D)$ I" where I is the body of the procedure and D is a sequence of variable declarations specifying the parameters of *foo*. A call of *foo* has the form $foo(P)$ where P is a parameter list. The parameter list has the same length as the variable declaration list. Parameter passing is either "by value" or "by reference". Our default assumption is that basic objects such as integers and boolean are passed by value and that complex objects such as arrays are passed by reference. These conventions are similar to the conventions used by C and guarantee that parameter passing takes constant time. The semantics of parameter passing is defined as follows: for a value parameter x of type T the actual parameter must be an expression E of type T and parameter passing is equivalent to the declaration $x = E\ : T$ and for a reference parameter x of type T, the actual parameter must be a variable of type T and the formal parameter is simply an alternative name for the actual parameter. As for variable declarations, we sometimes omit type declarations for parameters if they are unimportant or clear from the context. Sometimes we also declare parameters implicitly using mathematical notation. For example, the declaration **Procedure** $bar(\langle a_1, \ldots, a_n \rangle)$ introduces a procedure whose argument is a sequence of n elements of unspecified type.

Most procedure calls can be compiled into machine code by simply substituting the procedure body for the procedure call and making provisions for parameter passing; this is called *inlining*. Value passing is implemented by making appropriate assignments to copy the parameter values into the local variables of the procedure.

```
**Function** $factorial(n) : \mathbb{Z}$
    **if** $n = 1$ **then return** $1$ **else return** $n \cdot factorial(n-1)$
```

```
factorial :                                      // the first instruction of $factorial$
$R_n := RS[R_r - 1]$                             // load $n$ into register $R_n$
JZ thenCase, $R_n$                               // jump to then-case, if $n$ is zero
$RS[R_r] =$ aRecCall                             // else-case; return address for recursive call
$RS[R_r + 1] := R_n - 1$                         // parameter is $n - 1$
$R_r := R_r + 2$                                 // increase stack pointer
J factorial                                      // start recursive call
aRecCall :                                       // return address for recursive call
$R_{result} := RS[R_r - 1] * R_{result}$         // store $n * factorial(n-1)$ in result register
J return                                         // goto return
thenCase :                                       // code for then case
$R_{result} := 1$                                // put 1 into result register
return :                                         // code for return
$R_r := R_r - 2$                                 // free activation record
J $RS[R_r]$                                      // jump to return address
```

Fig. 2.2. A recursive function *factorial* and the corresponding RAM-code. The RAM-code returns the function value in register R_{result}.

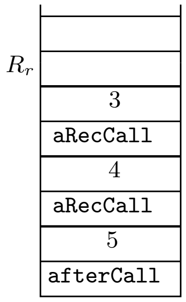


Fig. 2.3. The recursion stack of a call $factorial(5)$ when the recursion has reached $factorial(3)$.

Reference passing to a formal parameter $x : T$ is implemented by changing the type of x to **Pointer to** T, replacing all occurrences of x in the body of the procedure by $(*x)$ and initializing x by the assignment $x :=$ **addressof** y, where y is the actual parameter. Since the compiler subsequently has many opportunities for optimization, inlining is the most efficient approach for small procedures and procedures that are only called from a single place.

[Rewrap figure 2.3.] *Functions* are similar to procedures except that they allow ⟸ the return statement to return a value. Figure 2.2 shows the declaration of a recursive function that returns $n!$ and its translation into RAM-code. The substitution approach fails for *recursive* procedures and functions that directly or indirectly call themselves

— substitution would never terminate. Realizing recursive procedures in RAM-code requires the concept of a *recursion stack* r. It is not only used for recursive procedures but also for procedures where inlining is inappropriate for other reasons, e.g., because it would lead to a large increase in code size. The recursion stack is a reserved part of the memory; we use RS to denote it. RS contains a sequence of so-called *activation records*, one for each active procedure call. A special register R_r always points to the first free entry on this stack. The activation record for a procedure with k parameters and ℓ local variables has size $1 + k + \ell$. The first location contains the return address, i.e., the address of the instruction where execution is to be continued after the call has terminated, the next k locations are reserved for the parameters, and the final ℓ locations are for the local variables. A procedure call is now implemented as follows. First, the calling procedure $caller$ pushes the return address and the actual parameters onto the stack, increases R_r accordingly, and jumps to the first instruction of the called routine $called$. It reserves space for its local variables by increasing R_r accordingly. Then the body of *called* is executed. During execution of the body, any access to the i-th formal parameter ($0 \leq i < k$) is an access to $RS[R_r - \ell - k + i]$ and any access to the i-th local variable ($0 \leq i < \ell$) is an access to $RS[R_r - \ell + i]$. When *called* executes a **return** statement, it decreases R_r by $1 + k + \ell$ (observe that *called* knows k and ℓ) and execution continues at the return address (which can be found at $RS[R_r]$). Thus control is returned to $caller$. Note that recursion is no problem with this scheme since each incarnation of a routine will have its own stack area for its parameters and local variables. Figure 2.3 shows the content of the recursion stack of a call $factorial(5)$ when the recursion has reached $factorial(3)$. The label `afterCall` is the address of the instruction following the call $factorial(5)$ and `aRecCall` is defined in Figure 2.2.

Exercise 13 (Sieve of Eratosthenes). Translate the following pseudocode for finding all prime numbers up to n into RAM machine code. Argue correctness first.

```
$a = \langle 1, \ldots, 1 \rangle$ : $Array$ $[2..n]$ of $\{0, 1\}$ // if $a[i]$ is false, $i$ is known to be non-prime
for $i := 2$ to $\lfloor \sqrt{n} \rfloor$ do
    if $a[i]$ then for $j := 2i$ to $n$ step $i$ do  $a[j] := 0$
                        // if $a[i]$ is true, $i$ is prime and all multiples of $i$ are non-prime
for $i := 2$ to $n$ do  if $a[i]$ then output "$i$ is prime"
```

We also need a simple form of object oriented programming so that we can separate the interface and implementation of data structures. We will introduce our notation by way of example. The definition

```
Class $Complex(x, y : Element)$ of $Number$
    $Number$ $r := x$
    $Number$ $i := y$
    Function $abs$ : $Number$ return $\sqrt{r^2 + i^2}$
    Function $add(c' : Complex) : Complex$   return $Complex(r + c'.r, i + c'.i)$
```

gives a (partial) implementation of a complex number type that can use arbitrary numeric types for real and imaginary parts. Very often, our class names will begin

```
Function power($a : \mathbb{R}$; $n_0 : \mathbb{N}$) : $\mathbb{R}$
    assert $n_0 \geq 0$ and $\neg(a = 0 \wedge n_0 = 0)$          // It is not so clear what $0^0$ should be
    $p = a : \mathbb{R}$;   $r = 1 : \mathbb{R}$;   $n = n_0 : \mathbb{N}$          // we have: $p^n r = a^{n_0}$
    while $n > 0$ do
        invariant $p^n r = a^{n_0}$
        if $n$ is odd then $n--$; $r := r \cdot p$          // invariant violated between assignments
        else $(n, p) := (n/2, p \cdot p)$          // parallel assignment maintains invariant
    assert $r = a^{n_0}$          // This is a consequence of the invariant and $n = 0$
    return $r$
```

Fig. 2.4. An algorithm that computes integer powers of real numbers.

with capital letters. The real and imaginary parts are stored in the *member variables* r and i respectively. Now, the declaration "$c : \mathit{Complex}(2,3)$ **of** $\mathbb{R}$" declares a complex number c initialized to $2+3i$; $c.i$ is the imaginary part, and $c.\mathit{abs}$ returns the absolute value of c.

The type after the **of** allows us to parameterize classes with types in a way similar to the template mechanism of C++ or the generic types of Java. Note that in the light of this notation, the previously mentioned types "Set **of** $\mathit{Element}$" and "$\mathit{Sequence}$ **of** $\mathit{Element}$" are ordinary classes. Objects of a class are initialized by setting the member variables as specified in the class definition.

2.4 Designing Correct Algorithms and Programs

An algorithm is a general method for solving problems of a certain kind. We describe algorithms using natural language and mathematical notation. Algorithms as such cannot be executed by a computer. The formulation of an algorithm in a programming language is called a program. Designing correct algorithms and translating a correct algorithm into a correct program are non-trivial and error-prone tasks. In this section we learn about assertions and invariants, two useful concepts for the design of correct algorithms and programs.

Assertions and *invariants* describe properties of the program state, i.e., properties of single variables and relations between the values of several variables. Typical properties are: a pointer has a defined value, an integer is non-negative, a list is non-empty, or the value of an integer variable length is equal to the length of a certain list L. Figure 2.4 shows an example of the use of assertions and invariants in a function $\mathit{power}(a, n_0)$ that computes a^{n_0} for a real number a and a non-negative integer n_0.

We start with the assertion **assert** $n_0 \geq 0$ and $\neg(a = 0 \wedge n_0 = 0)$. It states that the program expects a non-negative integer n_0 and that not both a and n_0 are allowed to be zero. We make no claim about the behavior of our program for inputs violating the assertion. For this reason, the assertion is called the *precondition* of the program. It is good programming practice to check the precondition of a program, i.e., to write code which checks the precondition and signals an error if it is violated.

When the precondition holds (and the program is correct), the *postcondition* holds at termination of the program. In our example, we assert that $r = a^{n_0}$. It is also good programming practice to verify the postcondition before returning from a program. We come back to this point at the end of the section.

One can view preconditions and postconditions as a *contract* between the caller and the called routine: If the caller passes parameters satisfying the precondition, the routine produces a result satisfying the postcondition.

For conciseness, we will use assertions sparingly assuming that certain "obvious" conditions are implicit from the textual description of the algorithm. Much more elaborate assertions may be required for safety critical programs or even formal verification.

Pre- and postconditions are assertions describing the initial and the final state of a program or function. We also need to describe properties of intermediate states. Some particularly important consistency properties should hold at many places in the program. They are called *invariants*. Loop invariants and data structure invariants are of particular importance.

A *loop invariant* holds before and after each loop iteration. In our example, we claim $p^n r = a^{n_0}$ before each iteration. This is certainly true before the first iteration by the way the program variables are initialized. In fact, the invariant frequently tells us how to initialize the variables. Assume the invariant holds before execution of the loop body and $n > 0$. If n is odd, we decrement n and multiply r by p. This re-establishes the invariant. However, the invariant is violated between the assignments. If n is even, we halve n and square p and again re-establish the invariant. When the loop terminates, we have $p^n r = a^{n_0}$ by the invariant and $n = 0$ by the condition of the loop. Thus $r = a^{n_0}$ and we have established the postcondition.

Algorithm 2.4 and many more algorithms explained in this book have a quite simple structure: A couple of variables are declared and initialized to establish the loop invariant. Then a main loop manipulates the state of the program. When the loop terminates, the loop invariant together with the termination condition of the loop imply that the correct result has been computed. The loop invariant therefore plays a pivotal role in understanding why a program works correctly. Once we understand the loop invariant, it suffices to check that the loop invariant is true initially and after each loop iteration. This is particularly easy if the loop body consists of only a small number of statements as in the example above.

More complex programs encapsulate their state in objects whose consistent representation is also governed by invariants. Such *data structure invariants* are declared together with the data type. They are true after an object is constructed and they are preconditions and postconditions of all methods of the class. For example, we will discuss the representation of sets by sorted arrays. The data structure invariant will state that the data structure uses an array a and an integer n, that n is the size of a, that the set S stored in the data structure is equal to $\{a[1], \ldots, a[n]\}$ and that $a[1] < a[2] < \ldots < a[n]$. The methods of the class have to maintain this invariant and they are allowed to leverage the invariant, e.g., the search method may make use of the fact that the array is sorted.

We mentioned above that it is good programming practice to check assertions. It is not always clear how to do this efficiently; in our example program, it is easy to check the precondition, but there seems to be no easy way to check the postcondition. In many situations, however, *the task of checking assertions can be simplified by computing additional information*. The additional information is called a *certificate* or *witness* and its purpose it to simplify the check of an assertion. When an algorithm computes a certificate for the postcondition, we call it a *certifying algorithm*. We illustrate the idea by an example. Consider a function whose input is a graph $G = (V, E)$. Graphs are defined in Section 2.9. The task is to test whether the graph is bipartite, i.e., whether there is a labelling of the vertices of G with colors blue and red such that any edge of G connects vertices of distinct colors. As stated, the function returns true or false, true if G is bipartite and false otherwise. With this rudimentary output, the postcondition cannot be checked. However, we may augment the program as follows. When the program declares G bipartite, it also returns a two-coloring of the graph. When the program declares G non-bipartite, it also returns a cycle of odd length in the graph. For the augmented program, the postcondition is easy to check. In the first case, we simply check whether all edges connect vertices of distinct colors and in the second case, we do nothing. An odd length cycle proves that the graph is non-bipartite. Most algorithms in this book can be made certifying without increasing asymptotic running time.

2.5 An Example — Binary Search

Binary search is a very useful technique for searching in an ordered set of items. We will use it over and over again in later chapters.

The most simple scenario is as follows: We are given a sorted array $a[1..n]$ of elements, i.e., $a[1] < a[2] < \ldots < a[n]$, and an element x and are supposed to find the index i with $a[i-1] < x \leq a[i]$; here $a[0]$ and $a[n+1]$ should be interpreted as fictitious elements with value $-\infty$ and $+\infty$, respectively. We can use the fictitious elements in the invariants and the proofs, but cannot access them in the program.

Binary search is based on the principle of divide-and-conquer. We choose an index $m \in [1..n]$ and compare x and $a[m]$. If $x = a[m]$ we are done and return $i = m$. If $x < a[m]$, we restrict the search to the part of the array before $a[m]$, and if $x > a[m]$, we restrict the search to the part of the array after $a[m]$. We need to say more clearly what it means to restrict the search to a subinterval. We have two indices ℓ and r into the array and maintain the invariant

$$(I) \qquad 0 \leq \ell < r \leq n+1 \quad \text{and} \quad a[\ell] < x < a[r] \,.$$

This is true initially with $\ell = 0$ and $r = n + 1$. If ℓ and r are consecutive indices, x is not contained in the array. Figure 2.5 shows the complete program.

The comments in the program show that the second part of the invariant is maintained. With respect to the first part, we observe that the loop is entered with $\ell < r$. If $\ell + 1 = r$, we stop and return. Otherwise, $\ell + 2 \leq r$ and hence $\ell < m < r$. Thus

```
$(\ell, r) := (0, n+1)$
while $true$ do
    invariant $I$                                  // i.e., Invariant $(I)$ holds here
    if $\ell + 1 = r$ then return "$a[\ell] < x < a[\ell + 1]$"
    $m := \lfloor (r+\ell)/2 \rfloor$                                      // $\ell < m < r$
    $s := compare(x, a[m])$          // $-1$ if $x < a[m]$, $0$ if $x = a[m]$, $+1$ if $x > a[m]$
    if $s = 0$ then return "$x$ is equal to $a[m]$";
    if $s < 0$
        then $r := m$                              // $a[\ell] < x < a[m] = a[r]$
        else $\ell := m$                           // $a[\ell] = a[m] < x < a[r]$
```

Fig. 2.5. Binary Search for x in a sorted array $a[1..n]$

m is a legal array index and we can access $a[m]$. If $x = a[m]$, we stop. Otherwise, we either set $r = m$ or $\ell = m$ and hence have $\ell < r$ at the end of the loop. Thus the invariant is maintained.

Let us argue termination next. We observe first, that if an iteration is not the last then we either increase ℓ or decrease r and hence $r - \ell$ decreases. Thus the search terminates. We want to show more. We want to show that the search terminates in a logarithmic number of steps. We study the quantity $r - \ell - 1$. Note that this is the number of indices i with $\ell < i < r$ and hence a natural measure of the size of the current subproblem. If an iteration is not the last, this quantity decreases to

$$\begin{aligned}
&\max(r - \lfloor (r+\ell)/2 \rfloor - 1, \lfloor (r+\ell)/2 \rfloor - \ell - 1) \\
&\quad \le \max(r - ((r+\ell)/2 - 1/2) - 1, (r+\ell)/2 - \ell - 1) \\
&\quad = \max((r - \ell - 1)/2, (r-\ell)/2 - 1) = (r - \ell - 1)/2 \; ,
\end{aligned}$$

and hence it at least halved. We start with $r - \ell - 1 = n + 1 - 0 - 1 = n$ and hence have $r - \ell - 1 \le \lfloor n/2^k \rfloor$ after k iterations. The $(k+1)$-th iteration is certainly the last, if we enter it with $r = \ell + 1$. This is guaranteed if $n/2^k < 1$ or $k > \log n$. We conclude that at most $2 + \log n$ iterations are performed. Since the number of comparisons is a natural number, we can sharpen the bound to $2 + \lfloor \log n \rfloor$.

Theorem 4. *Binary search finds an element in a sorted array in* $2 + \lfloor \log n \rfloor$ *comparisons between elements.*

Exercise 14. Show that the bound is sharp, i.e., for every n there are instances where exactly $2 + \lfloor \log n \rfloor$ comparisons are needed.

Exercise 15. Formulate binary search with two-way comparisons, i.e., distinguish between the cases $x < a[m]$, and $x \ge a[m]$.

We next discuss two important extensions of binary search. First, there is no need for the values $a[i]$ to be stored in an array. We only need the capability to compute $a[i]$ given i. For example, if we have a strictly monotone function f and arguments i and j with $f(i) < x < f(j)$, we can use binary search to find m with

$f(m) \leq x < f(m+1)$. In this context, binary search is often referred to as the *bisection method*.

Second, we can extend binary search to the case that the array is infinite. Assume we have an infinite array $a[1..\infty]$ with $a[1] \leq x$ and want to find m such that $a[m] \leq x < a[m+1]$. If x is larger than all elements in the array, the procedure is allowed to diverge. We proceed as follows. We compare x with $a[2^1]$, $a[2^2]$, $a[2^3]$, $\ldots$, until the first i with $x < a[2^i]$ is found. This is called an *exponential search*. Then we complete the search by binary search on the array $a[2^{i-1}..2^i]$.

Theorem 5. *Exponential and binary search finds x in an unbounded sorted array in $2\log m + 3$ comparisons, where $a[m] \leq x < a[m+1]$.*

Proof. We need i comparisons to find the first i with $x < a[2^i]$ and then $\log(2^i - 2^{i-1}) + 2$ comparisons for the binary search. This makes $2i + 1$ comparisons. Since $m \geq 2^{i-1}$ we have $i \leq 1 + \log m$ and the claim follows.

Binary search is certifying. It returns an index m with $a[m] \leq x < a[m+1]$. If $x = a[m]$, the index proves that x is stored in the array. If $a[m] < x < a[m+1]$ and the array is sorted, the index proves that x is not stored in the array. Of course, if the array violates the precondition and is not sorted, we know nothing. There is no way to check the precondition in logarithmic time.

2.6 Basic Program Analysis

Let us summarize the principles of program analysis. We abstract from the complications of a real machine to the simplified RAM model. In the RAM model, running time is measured by the number of instructions executed. We simplify further by grouping inputs by size and focussing on the worst case. The use of asymptotic notation allows us to ignore constant factors and lower order terms. This coarsening of our view also allows us to look at upper bounds on the execution time rather than the exact worst case as long as the asymptotic result remains unchanged. The total effect of these simplifications is that the running time of pseudocode can be analyzed directly. There is no need for translating into machine code first.

We will next introduce a set of simple rules for analyzing pseudocode. Let $T(I)$ denote the worst case execution time of a piece of program I. Then the following rules tell us how to estimate running time for larger programs given that we know the running time of their constituents:

- $T(I; I') = T(I) + T(I')$.
- $T($**if** C **then** I **else** $I') = \mathcal{O}(T(C) + \max(T(I), T(I')))$.
- $T($**repeat** I **until** $C) = \mathcal{O}\left(\sum_{i=1}^{k} T(i)\right)$ where k is the number of loop iterations, and where $T(i)$ is the time needed in the i-th iteration of the loop.

We postpone the treatment of subroutine calls to Section 2.6.2. Among the rules above, only the rule for loops is non-trivial to apply. It requires evaluating sums.

2.6.1 “Doing Sums”

We introduce basic techniques for evaluating sums. Sums arise in the analysis of loops, in average case analysis, and also in the analysis of randomized algorithms.

For example, the insertion sort algorithm introduced in Section 5.1 has two nested loops. The outer loop counts i from 2 to n. The inner loop performs at most $i-1$ iterations. Hence, the total number of iterations of the inner loop is at most

$$\sum_{i=2}^{n}(i-1)=\sum_{i=1}^{n-1} i=\frac{n(n-1)}{2}=\mathcal{O}\big(n^2\big)\ ,$$

where the second equality is Equation $(A.11)$. Since the time for one execution of the inner loop is $\mathcal{O}(1)$, we get a worst case execution time of $\Theta\big(n^2\big)$. All nested loops with an easily predictable number of iterations can be analyzed in an analogous fashion: Work your way inside out by repeatedly finding a closed form expression for the innermost loop. Using simple manipulations like $\sum_i ca_i = c\sum_i a_i$, $\sum_i(a_i+b_i)=\sum_i a_i+\sum_i b_i$, or $\sum_{i=2}^{n} a_i=-a_1+\sum_{i=1}^{n} a_i$ one can often reduce the sums to simple forms that can be looked up in a catalogue of sums. A small sample of such formulae can be found in Appendix A. Since we are usually only interested in the asymptotic behavior, we can frequently avoid doing sums exactly and resort to estimates. For example, instead of evaluating the sum above exactly, we may argue more simply:

$$\begin{aligned}\sum_{i=2}^{n}(i-1) &\le \sum_{i=1}^{n} n = n^2=\mathcal{O}\big(n^2\big)\\ \sum_{i=2}^{n}(i-1) &\ge \sum_{i=\lceil n/2\rceil}^{n} n/2=\lfloor n/2\rfloor\cdot n/2=\Omega\big(n^2\big)\ .\end{aligned}$$

2.6.2 Recurrences

In our rules for analyzing programs we have so far neglected subroutine calls. Nonrecursive subroutines are easy to handle since we can analyze the subroutine separately and then substitute the obtained bound into the expression for the running time of the calling routine. For recursive programs this approach does not lead to a closed formula, but to a recurrence relation.

For example, for the recursive variant of school multiplication, we obtained $T(1)=1$ and $T(n)=6n+4T(\lceil n/2\rceil)$ for the number of primitive operations. For the Karatsuba algorithm, the corresponding expression was $T(n)=3n^2+2n$ for $n\le 3$ and $T(n/2)=12n+3T(\lceil n/2\rceil+1)$ otherwise. In general, a *recurrence relation* defines a function in terms of the same function using smaller arguments. Explicit definitions for small parameter values make the function well defined. Solving recurrences, i.e., giving non-recursive, closed form expressions for them is an interesting subject of mathematics. Here we focus on recurrence relations that typically emerge from divide-and-conquer algorithms. We begin with a simple case that

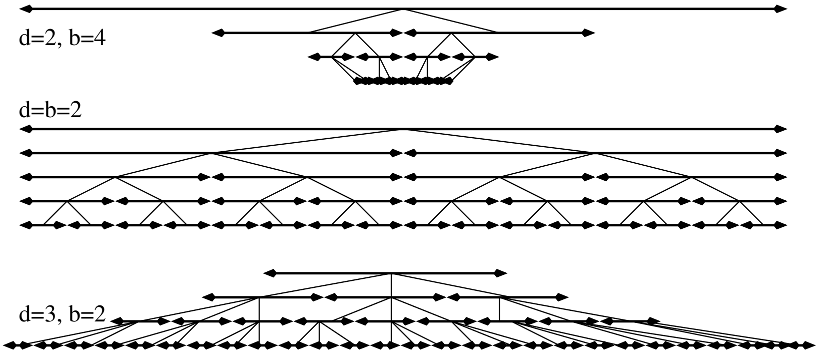


Fig. 2.6. Examples for the three cases of the master theorem. Problems are indicated by horizontal segments with arrows on both ends. The length of a segment represents the size of the problem and the subproblems resulting from a problem are shown in the next line. The topmost figure corresponds to the case $d = 2$ and $b = 4$, i.e., each problem generates 2 subproblems of one-fourth the size. Thus the total size of the subproblems is only half of the original size. The middle figure illustrates the case $d = b = 2$ and the bottommost figure illustrates the case $d = 3$ and $b = 2$.

already suffices to understand the main ideas. We have a problem of size $n = b^k$ and integer k. If $k > 1$, we invest linear work cn on dividing the problem and combining the results of the subproblems and generate d subproblems of size n/b. If $k = 0$, there are no recursive calls, we invest work a and are done.

Theorem 6 (Master Theorem (Simple Form)). *For positive constants a, b, c, and d, and $n = b^k$ for some integer k, consider the recurrence*

$$r(n) = \begin{cases} a & \text{if } n = 1 \\ cn + d \cdot r(n/b) & \text{if } n > 1 \ . \end{cases}$$

Then

$$r(n) = \begin{cases} \Theta(n) & \text{if } d < b \\ \Theta(n \log n) & \text{if } d = b \\ \Theta\big(n^{\log_b d}\big) & \text{if } d > b \ . \end{cases}$$

Figure 2.6 illustrates the main insight behind Theorem 6: We consider the amount of work done at each level of recursion. We start with a problem of size n. At the i-th level of the recursion we have d^i problems each of size n/b^i. Thus the total size of the problems at the i-th level is equal to

$$d^i \frac{n}{b^i} = n \left(\frac{d}{b}\right)^i \ .$$

The work performed for a problem is c times the problem size and hence the work performed on a certain level of the recursion is proportional to the total problem size on that level. Depending on whether d/b is smaller, equal, or larger than 1, we have different kinds of behavior.

If $d < b$, the work *decreases geometrically* with the level of recursion and the *first* level of recursion already accounts for a constant fraction of total execution time.

If $d = b$, we have the same amount of work at *every* level of recursion. Since there are logarithmically many levels, the total amount of work is $\Theta(n \log n)$.

Finally, if $d > b$ we have a geometrically *growing* amount of work in each level of recursion so that the *last* level accounts for a constant fraction of the total running time. We next formalize this reasoning.

Proof. We start with a single problem of size $n = b^k$. Call this level zero of the recursion. At level one, we have d problems each of of size $n/b = b^{k-1}$. At level two, we have d^2 problems each of size $n/b^2 = b^{k-2}$. At level i, we have d^i problems each of size $n/b^i = b^{k-i}$. At level k, we have d^k problems each of size $n/b^k = b^{k-k} = 1$. Each such problem has cost a and hence the total cost at level k is ad^k.

Let us next compute the total cost of the divide-and-conquer steps in levels 1 to $k-1$. At level i, we have d^i recursive calls each for subproblems of size b^{k-i}. Each call contributes a cost of $c \cdot b^{k-i}$ and hence the cost at level i is $d^i \cdot c \cdot b^{k-i}$. Thus the combined cost over all levels is

$$\sum_{i=0}^{k-1} d^i \cdot c \cdot b^{k-i} = c \cdot b^k \cdot \sum_{i=0}^{k-1} \left(\frac{d}{b}\right)^i = cn \cdot \sum_{i=0}^{k-1} \left(\frac{d}{b}\right)^i \quad .$$

We now distinguish cases according to the relative size of d and b.

Case $d = b$**:** We have cost $ad^k = ab^k = an = \Theta(n)$ for the bottom of the recursion and $cnk = cn \log_b n = \Theta(n \log n)$ for the divide-and-conquer steps.

Case $d < b$**:** We have cost $ad^k < ab^k = an = \mathcal{O}(n)$ for the bottom of the recursion. For the cost of the divide-and-conquer steps we use Formula A.13 for a geometric series, namely $\sum_{0 \le i < k} x^i = (1 - x^k)/(1 - x)$ for $x > 0$ and $x \neq 1$, and obtain

$$cn \cdot \sum_{i=0}^{k-1} \left(\frac{d}{b}\right)^i = cn \cdot \frac{1 - (d/b)^k}{1 - d/b} < cn \cdot \frac{1}{1 - d/b} = \mathcal{O}(n)$$

and

$$cn \cdot \sum_{i=0}^{k-1} \left(\frac{d}{b}\right)^i = cn \cdot \frac{1 - (d/b)^k}{1 - d/b} > cn = \Omega(n) \quad .$$

Case $d > b$**:** First note that

$$d^k = 2^{k \log d} = 2^{k \frac{\log b}{\log b} \log d} = b^{k \frac{\log d}{\log b}} = b^{k \log_b d} = n^{\log_b d} \quad .$$

Hence the bottom of the recursion has cost $an^{\log_b d} = \Theta\big(n^{\log_b d}\big)$. For the divide-and-conquer steps we use the geometric series again and obtain

$$cb^k \frac{(d/b)^k - 1}{d/b - 1} = c\frac{d^k - b^k}{d/b - 1} = cd^k \frac{1 - (b/d)^k}{d/b - 1} = \Theta\big(d^k\big) = \Theta\big(n^{\log_b d}\big) \quad .$$

The recurrence $T(n) = 3n^2 + 2n$ for $n \leq 3$ and $T(n/2) = 12n + 3T(\lceil n/2 \rceil + 1)$ otherwise governing Karatsuba's algorithm is not covered by our master theorem. We will now show how to extend the master theorem to this situation: assume $r(n)$ is defined by $r(n) \leq a$ for $n \leq n_0$ and $r(n) \leq cn + d \cdot r(\lceil n/b \rceil + e)$ for $n > n_0$ where n_0 is such that $\lceil n/b \rceil + e < n$ for $n > n_0$ and a, b, c, d and e are constants. We proceed in two steps. We first concentrate on n of the form $b^k + z$ where z is such that $\lceil z/b \rceil + e = z$. For example, for $b = 2$ and $e = 3$, we would choose $z = 6$. Note that for n of this form we have $\lceil n/b \rceil + e = \lceil (b^k + z)/b \rceil + e = b^{k-1} + \lceil z/b \rceil + e = b^{k-1} + z$, i.e., the reduced problem size has the same form. For the n's in special form we then argue exactly as in Theorem 6.

How do we generalize to arbitrary n? The simplest way is semantic reasoning. It is clear[2] that it is more difficult to solve larger inputs than smaller inputs and hence the cost for input size n will be no larger than the time needed on an input whose size is equal to the next input size of special form. Since this input is at most b times larger and b is a constant, the bound derived for special n is only affected by a constant factor.

Formal reasoning is as follows (you may want to skip this paragraph and come back to it when need arises): We define a function $R(n)$ by the same recurrence with $\leq$ replaced by equality: $R(n) = a$ for $n \leq n_0$ and $R(n) = cn + dR(\lceil n/b \rceil + e)$ for $n > n_0$. Obviously, $r(n) \leq R(n)$. We derive a bound for $R(n)$ and n of special form as described above. Finally, we argue by induction that $R(n) \leq R(s(n))$ where $s(n)$ is the smallest number of the form $b^k + z$ with $b^k + z \geq n$. The induction step is as follows:

$$R(n) = cn + dR(\lceil n/b \rceil + e) \leq cs(n) + dR(s(\lceil n/b \rceil + e)) = R(s(n)) ,$$

where the inequality uses the induction hypothesis and $n \leq s(n)$ and the last equality uses the fact that for $s(n) = b^k + z$ and hence $b^{k-1} + z < n$ we have $b^{k-2} + z < \lceil n/b \rceil + e \leq b^{k-1} + z$ and hence $s(\lceil n/b \rceil + e) = b^{k-1} + z = \lceil s(n)/b \rceil + e$.

There are many generalizations of the Master Theorem: We might break the recursion earlier, the cost for dividing and conquering may be nonlinear, the size of the subproblems might vary within certain bounds, the number of subproblems may depend on the input size, etc. We refer the reader to the books [164, 79] for further information.

Exercise 16. Consider the recurrence $C(1) = 1$ and $C(n) = C(\lfloor n/2 \rfloor) + C(\lceil n/2 \rceil) + cn$ for $n > 1$. Show $C(n) = O(n \log n)$.

***Exercise 17** Suppose you have a divide-and-conquer algorithm whose running time is governed by the recurrence

$$T(1) = a, T(n) = cn + \left\lceil \sqrt{n} \right\rceil T(\lceil n / \left\lceil \sqrt{n} \right\rceil \rceil) \ .$$

Show that the running time of the program is $\mathcal{O}(n \log \log n)$.

[2] Be aware that most errors in mathematical arguments are near occurrences of the word 'clearly'.

Exercise 18. Access to data structures is often governed by the following recurrence: $T(1) = a$, $T(n) = c + T(n/2)$. Show $T(n) = \mathcal{O}(\log n)$.

2.6.3 Global Arguments

The program analysis techniques introduced so far are syntax-oriented in the following sense. In order to analyze a large program, we first analyze its parts and then combine the analyses of the parts to an analysis of the large program. The combine step involves sums and recurrences.

We will also use a completely different approach which one might call semantics-oriented. In this approach we associate parts of the execution with parts of a combinatorial structure and then argue about the combinatorial structure. For example, we might argue that a certain piece of program is executed at most once for each edge of a graph or that execution of a certain piece of program at least doubles the size of a certain structure, that the size is one initially, at most n at termination, and hence the number of executions is bounded logarithmically.

2.7 Average Case Analysis

In this section we will introduce you to average case analysis. We do so by way of three examples of increasing complexity. We assume that you are familiar with basic concepts of probability theory such as discrete probability distributions, expected values, indicator variables, and linearity of expectation. Appendix A.2 reviews the basics.

We come to our first example. Our input is an array $a[0..n-1]$ filled with digits zero and one. We want to increment the number represented by the array by one.

```
$i := 0$
**while** $(i < n$ *and* $a[i] = 1)$ **do** $a[i] = 0;\ i{+}{+};$
**if** $i < n$ **then** $a[i] = 1$
```

How often is the body of the while-loop executed? Clearly, n times in the worst case and 0 times in the best case. What is the average case? The first step in an average case analysis is always to define the model of randomness, i.e. to define the underlying probability space. We postulate the following model of randomness. Each digit is zero or one with probability $1/2$ and different digits are independent. The loop body is executed k times, $0 \le k \le n$, iff the last $k+1$ digits of a are 01^k or k is equal to n and all digits of a are equal to one. The former event has probability $2^{-(k+1)}$ and the latter event has probability 2^{-n}. Therefore, the average number of executions is equal to

$$\sum_{0 \le k < n} k2^{-(k+1)} + n2^{-n} \le \sum_{k \ge 0} k2^{-k} = 2\ ,$$

where the last equality is Equation (A.14).

Our second example is slightly more demanding. Consider the following simple program that determines the maximum element in an array $a[1..n]$.

```
$m := a[1]$    for $i := 2$ to $n$ do if $a[i] > m$ then $m := a[i]$
```

How often is the assignment $m := a[i]$ executed? In the worst case, it is executed in every iteration of the loop and hence $n-1$ times. In the best case, it is not executed at all. What is the average case? Again, we start by defining the probability space. We assume that the array contains n distinct elements and that any order of these elements is equally likely. In other words, our probability space consists of the $n!$ permutations of the array elements. Each permutation is equally likely and therefore has probability $1/n!$. Since the exact nature of the array elements is unimportant, we may assume that the array contains the numbers 1 to n in some order. We are interested in the average number of *left-to-right maxima*. A left-to-right maximum in a sequence is an element which is larger than all preceding elements. So $(1,2,4,3)$ has three left-to-right-maxima and $(3,1,2,4)$ has two left-to-right-maxima. For a permutation π of the integers 1 to n, let $M_n(\pi)$ be the number of left-to-right-maxima. What is $\mathrm{E}[M_n]$? We will describe two ways to determine the expectation. For small n, is easy to determine $\mathrm{E}[M_n]$ by direct calculation. For $n=1$, there is only one permutation, namely (1) and it has one maximum. So $\mathrm{E}[M_1]=1$. For $n=2$, there are two permutations, namely $(1,2)$ and $(2,1)$. The former has two maxima and the latter has one maximum. So $\mathrm{E}[M_2]=1.5$. For larger n, we argue as follows.

We write M_n as a sum of indicator variables I_1 to I_n, i.e., $M_n = I_1 + \ldots + I_n$ where I_k is equal to one for a permutation π if the k-th element of π is a left-to-right-maximum. For example, $I_3((3,1,2,4))=0$ and $I_4((3,1,2,4))=1$. We have

$$\begin{aligned}\mathrm{E}[M_n] &= \mathrm{E}[I_1 + I_2 + \ldots + I_n]\\ &= \mathrm{E}[I_1] + \mathrm{E}[I_2] + \ldots + \mathrm{E}[I_n]\\ &= \mathrm{prob}(I_1 = 1) + \mathrm{prob}(I_2 = 1) + \ldots + \mathrm{prob}(I_n = 1)\ ,\end{aligned}$$

where the second equality is linearity of expectations (Equation A.2) and the third equality follows from the I_k's being indicator variables. It remains to determine the probability that $I_k = 1$. The k-th element of a random permutation is a left-to-right maximum with probability $1/k$ because this is the case if and only if the k-th element is the largest of the first k elements. Since every permutation of the first k elements is equally likely, this probability is $1/k$. Thus $\mathrm{prob}(I_k = 1) = 1/k$ and hence

$$\mathrm{E}[M_n] = \sum_{1\le k\le n} \mathrm{prob}(I_k = 1) = \sum_{1\le k\le n} \frac{1}{k}\ .$$

So $\mathrm{E}[M_4] = 1 + 1/2 + 1/3 + 1/4 = (12+6+4+3)/12 = 25/12$. The sum $\sum_{1\le k\le n} 1/k$ will show up several times in this book. It is known under the name n-th harmonic number and is denoted H_n. It is known that $\ln n \le H_n \le 1 + \ln n$, i.e., $H_n \approx \ln n$; see Equation (A.12). We conclude that the average number of left-right maxima is much smaller than the worst case.

Exercise 19. Show that $\sum_{k=1}^{n} \frac{1}{k} \le \ln n + 1$. Hint: show first that $\sum_{k=2}^{n} \frac{1}{k} \le \int_1^n \frac{1}{x}\,dx$.

We come to an alternative analysis. Introduce A_n as a shorthand for $\mathrm{E}[M_n]$ and set $A_0 = 0$. The first element is always a left-to-right maximum and each number is equally likely as first element. If the first element is equal to i, then only the numbers $i + 1$ to n can be further left-to-right maxima. They appear in random order in the remaining sequence and hence we will see an expected number of A_{n-i} further maxima. Thus

$$A_n = 1 + \left(\sum_{1 \le i \le n} A_{n-i} \right) / n \qquad \text{or} \qquad nA_n = n + \sum_{1 \le i \le n-1} A_i \ .$$

The corresponding equation for $n - 1$ instead of n is $(n-1)A_{n-1} = n - 1 + \sum_{1 \le i \le n-2} A_i$. Subtracting both equations yields

$$nA_n - (n-1)A_{n-1} = 1 + A_{n-1} \qquad \text{or} \qquad A_n = 1/n + A_{n-1} \ ,$$

and hence $A_n = H_n$.

We come to our third example; this example is even more demanding. Consider the following searching problem. We have items 1 to n which we are supposed to arrange linearly in some order, say we put item i in position ℓ_i. Once we have arranged the items, we perform searches. In order to search for an item x, we go through the sequence from left to right until we encounter x. In this way, it will take ℓ_i steps to access item i.

Suppose now that we also know that we access the items with different probabilities, say we search for item i with probability p_i where $p_i \ge 0$ for all i, $1 \le i \le n$, and $\sum_i p_i = 1$. In this situation, the *expected or average cost of a search* is equal to $\sum_i p_i \ell_i$ since we search for item i with probability p_i and the cost of the search is ℓ_i.

What is the best way of arranging the items? Intuition tells us that we should arrange the items in order of decreasing probability. Let us prove this.

Lemma 7. *An arrangement is optimal with respect to expected search cost if it has the property that $p_i > p_j$ implies $\ell_i < \ell_j$. If $p_1 \ge p_2 \ge \ldots p_n$, the placement $\ell_i = i$ results in the optimal expected search cost $Opt = \sum_i p_i i$.*

Proof. Consider an arrangement in which for some i and j we have $p_i > p_j$ and $\ell_i > \ell_j$, i.e., item i is more probable than item j and yet placed after it. Interchanging items i and j changes the search cost by

$$-(p_i \ell_i + p_j \ell_j) + (p_i \ell_j + p_j \ell_i) = (p_i - p_j)(\ell_i - \ell_j) < 0 \ ,$$

i.e., the new arrangement is better and hence the old arrangement is not optimal.

Let us now consider the case $p_1 > p_2 > \ldots > p_n$. Since there are only $n!$ possible arrangements, there is an optimal arrangement. Also, if $i < j$ and i is placed after j, the arrangement is not optimal by the preceding paragraph. Thus the optimal arrangement puts item i in position $\ell_i = i$ and its expected search cost is $\sum_i p_i i$.

If $p_1 \ge p_2 \ge \ldots p_n$, the arrangement $\ell_i = i$ for all i is still optimal. However, if some probabilities are equal, we have more than one optimal arrangement. Within blocks of equal probabilities, the order is irrelevant.

Can we still do something intelligent, if the probabilities p_i are not known to us? The answer is yes and a very simple heuristic does the job. It is called the *move-to-front-heuristic*. Suppose we access item i and find it in position ℓ_i. If $\ell_i = 1$, we are happy and do nothing. Otherwise, we place it in position 1 and move the items in positions 1 to $\ell_i - 1$ one position to the rear. The hope is that in this way frequently accessed items tend to stay near the front of the arrangement and infrequently accessed items move to the rear. We next analyze the expected behavior of the move-to-front-heuristic.

Consider two items i and j and suppose both of them were accessed in the past. Item i will be before item j if the last access to item i occurred after the last access to item j. Thus the probability that item i is before item j is $p_i/(p_i + p_j)$. With probability $p_j/(p_i + p_j)$ item j stands before item i.

Now ℓ_i is simply one plus the number of elements before i in the list. Thus the expected value of ℓ_i is equal to $1 + \sum_{j;\, j \neq i} p_j/(p_i + p_j)$ and hence the expected search cost in the move-to-front-heuristic is

$$C_{MTF} = \sum_i p_i \Big(1 + \sum_{j;\, j\neq i} \frac{p_j}{p_i + p_j}\Big) = \sum_i p_i + \sum_{ij;\, i \neq j} \frac{p_i p_j}{p_i + p_j} \ .$$

Observe that for each i and j with $i \neq j$, the term $p_i p_j/(p_i + p_j)$ appears twice in the list above. In order to proceed in the analysis, we assume $p_1 \geq p_2 \geq \ldots \geq p_n$. This is an assumption used in the analysis, the algorithm has no knowledge of this. Then

$$\begin{aligned} C_{MTF} &= \sum_i p_i + 2 \sum_{j;\, j<i} \frac{p_i p_j}{p_i + p_j} = \sum_i p_i \Big(1 + 2 \sum_{j;\, j<i} \frac{p_j}{p_i + p_j}\Big) \\ &\leq \sum_i p_i \Big(1 + 2 \sum_{j;\, j<i} 1\Big) < \sum_i p_i 2i = 2 \sum_i p_i i = 2 Opt \ . \end{aligned}$$

Theorem 7. *The move-to-front-heuristic achieves an expected search time which is at most twice the optimum.*

2.8 Randomized Algorithms

Suppose you are offered to participate in a TV game show: There are 100 boxes that you can open in an order of your choice. Box i contains an amount m_i of money. The amount is unknown to you and becomes known once the box is opened. No two boxes contain the same amount of money. The rules of the game are very simple.

- At the beginning of the game, the show master gives you 10 tokens.
- When you open a box and the content of the box is larger than the content of all previously opened boxes, you have to hand back a token[3].

[3] The content of the first box opened is larger than the content of all previously opened boxes and hence the first token goes back to the show master in the first round.

- When you have to hand back a token, but have no token, the game ends and you loose.
- When you manage to open all boxes, you win and can keep all the money.

There are strange pictures on the boxes and the show master gives hints by suggesting the box to be opened next. Your Aunt, who is addicted to this show, tells you that only few candidates win. Now you ask yourself whether it is worth participating in this game. Is there a strategy that gives you a good chance to win? Are the hints of the show master useful?

Let us first analyze the obvious algorithm — you always follow the show master. The worst case is that he makes you open the boxes in order of increasing weight. Whenever you open a box, you have to hand back a token and when you open the 11-th box you are dead. The candidates and viewers would hate the show master and he would be fired soon. Worst case analysis does not give us the right information in this situation. The best case is that the show master immediately tells you the best box. You would be happy but there would be no time to place advertisements so that the show master would again be fired. Best case analysis also does not give us the right information in this situation. We next observe that the game is really the left-right maxima question of the preceding section in disguise. You have to hand back a token whenever a new maximum shows up. We saw in the preceding section that the expected number of left-right maxima in a random permutation is H_n, the n-th harmonic number. For $n = 100$, $H_n < 6$. So if the show master would point to the boxes in random order, on average, you would have to hand back only 6 tokens. But, why should the show master offer you the boxes in random order? He has no incentive to have too many winners.

The solution is to take your fate in your own hands: *open the boxes in random order*. You select one of the boxes at random, open it, then choose a random box among the remaining ones, and so on. How do you chose a random box? When there are k boxes left, you choose a random box by tossing a die with k sides or by choosing a random number in the range 1 to k. In this way, you generate a random permutation of the boxes and hence the analysis from the previous section still applies. On average you will have to return less than 6 tokens and hence your ten tokens suffice. You have just seen a *randomized algorithm*. We want to stress that, although the mathematical analysis is the same, the conclusions are very different. In the average case scenario, you are at the mercy of the show master. If he opens the boxes in random order, the analysis applies, if he does not, it does not. You have no way to tell except after many shows and in hindsight. In other words, the show master controls the dices and it is up to him whether he uses a fair dice. The situation is completely different in the randomized algorithms scenario. You control the dices and you generate the random permutation. The analysis is valid no matter what the show master does.

Formally, we equip our RAM with an additional instruction: $R_i := \mathit{randInt}(C)$ assigns a *random* integer between 0 and $C - 1$ to R_i. In Pseudocode we write $v := \mathit{randInt}(C)$, where v is an integer variable. The cost of making a random choice is one time unit.

The running time of a randomized algorithm will generally depend on the random choices made by the algorithm. So the running time on an instance i is no longer a number, but a random variable depending on the random choices. We may eliminate the dependency of the running time on random choices by equipping our machine with a timer. At the beginning of the execution, we set the timer to a value $T(n)$, say depending on the size n of the problem instance, and stop the machine once the timer goes off. In this way, we can guarantee that the running time is bounded by $T(n)$. However, if the algorithm runs out of time, it does not deliver an answer.

The output of a randomized algorithm may also depend on the random choices made. How can an algorithm be useful, if the answer on an instance i may depend on the random choices made by the algorithm? If the answer is "Yes" today and maybe "No" tomorrow. If the two cases are equally probable, the answer given by the algorithm has no value. However, if the correct answer is much more likely than the incorrect answer, the answer does have value. Let us see an example.

Alice and Bob are connected over a slow telephone line. Alice has an integer x_A and Bob has an integer x_B, each with n bits. They want to determine whether they have the same number. They could send the digits in turn. In the worst-case they will have to transmit n digits. Alternatively, they might do the following. Each one of them prepares an ordered list of prime numbers. The list consists of the smallest L primes with k or more bits. We say more about the choice of L and k below. In this way, it is guaranteed that they both generate the same list. Then Alice chooses a index i, $1 \leq i \leq L$, at random and sends i and $x_A \bmod p_i$ to Bob. Bob computes $x_B \bmod p_i$. If $x_A \bmod p_i \neq x_B \bmod p_i$, he declares that the numbers are different. Otherwise, he declares the numbers the same. Clearly, if the numbers are the same, Bob will say so. If the number are different and $x_A \bmod p_i \neq x_B \bmod p_i$, he will declare them different. However, if $x_A \neq x_B$ and yet $x_A \bmod p_i = x_B \bmod p_i$, he will erroneously declare the numbers equal. What is the probability of an error?

An error occurs if $x_A \neq x_B$ and yet $x_A \bmod p_i = x_B \bmod p_i$. The latter condition is equivalent to p_i dividing the difference $x_A - x_B$. The difference is at most 2^n in absolute value. Since each prime p_i has value at least 2^k, our list contains at most n/k primes that divide the difference. So the probability of error is at most $(n/k)/L$. We can make this probability arbitrarily small by choosing L large enough. Say, we want to make the probability to be less than $0.0000001 = 10^{-6}$. We choose $L = 10^6(n/k)$.

How many bits will the protocol transmit? Out of the numbers with k bits, approximately $2^k/k$ are primes[4]. Hence, if $2^k/k \geq 10^6 n/k$, the list will only contain k-bit integers. The condition $2^k \geq 10^6 n$ is tantamount to $k \geq \log n + 6 \log 10$. Thus the protocol transmits $\log L + k = \log n + 12 \log 10$ bits. This is exponentially better than the naive protocol.

[4] For any integer x, let $\pi(x)$ be the number of primes less than or equal to x. For example, $\pi(10) = 4$ because there are four prime numbers (2, 3, 5 and 7) less than or equal to 10. Then $\frac{x}{\ln x + 2} < \pi(x) < \frac{x}{\ln x - 4}$ for $x \geq 55$. See the Wikipedia entry on prime numbers for more information.

What can we do if we want error probability less than 10^{-12}. We could redo the calculations above with $L = 10^{12}n$. Alternatively, we could run the protocol twice and declare the numbers different if at least one run declares them different. The two-stage protocol errs only if both runs err and hence the probability of error is at most $10^{-6} \cdot 10^{-6} = 10^{-12}$.

Exercise 20. Compare the efficiency of the two approaches for obtaining error probability 10^{-12}.

Exercise 21. Assume you have an algorithm which errs with probability at most $1/4$. Run the algorithm k times and output the majority output. Derive a bound on the error probability as a function of k. Do a precise calculation for $k = 2$ and $k = 3$ and give a bound for large k. Finally, determine k such that the error probability is less than a given ϵ.

Randomized algorithms come in two main varieties, the Las Vegas and the Monte Carlo variety. A *Las Vegas algorithm* always computes the correct answer but its running time is a random variable. Our solution for the game show is a Las Vegas algorithm; it always finds the box containing the maximum; however, the number of left-right maxima is a random variable. A *Monte Carlo* algorithm always has the same run time yet there is a nonzero probability that it gives an incorrect answer. The probability that the answer is incorrect is at most 1/4. Our algorithm for comparing two numbers over a telephone line is a Monte Carlo algorithm. In Exercise 21 it is shown that the error probability can be made arbitrarily small.

Exercise 22. Suppose you have a Las Vegas algorithm with expected execution time $t(n)$. Run it for $4t(n)$ steps. If it returns an answer within the alloted time, return the answer. Otherwise return an arbitrary answer. Show that the resulting algorithm is a Monte Carlo algorithm.

Exercise 23. Suppose you have a Monte Carlo algorithm with execution time $m(n)$ that gives a correct answer with probability p and a deterministic algorithm that verifies in time $v(n)$ whether the Monte Carlo algorithm has given the correct answer. Explain how to use these two algorithms to obtain a Las Vegas algorithm with expected execution time $\frac{1}{1-p}(m(n) + v(n))$.

We come back to our game show example. You have ten tokens available to you. The expected number of tokens required is less than 6. How sure should you be that you go home as a winner? We need to bound the probability that M_n is larger than 11, because you loose exactly if the sequence in which you order the boxes has 11 or more left-right maxima. The so-called *Tschebyscheff inequality* allows to bound this probability. It states, that for a non-negative random variable X and any constant $c \geq 1$, $\text{prob}(X \geq c \cdot \text{E}[X]) \leq 1/c$; see Equation (**??**) for additional information. We apply the inequality with $X = M_n$, and $c = 11/6$. Then

$$\text{prob}(M_n \geq 11) \leq \text{prob}(M_n \geq \frac{11}{6}\text{E}[M_n]) \leq \frac{6}{11} ,$$

and hence the probability to win is more than 5/11.

2.9 Graphs

Graphs are an extremely useful concept in algorithmics. We use them whenever we want to model objects and relations between them; in graph terminology, the objects are called *nodes* and the relation between nodes are called *edges*. Obvious applications are road maps or communication networks, but there are also more abstract applications. For example, nodes could be tasks to be completed when building a house like "build the walls" or "put in the windows" and edges model precedence relations like "the walls have to be built before the windows can be put in". We will also see many examples of data structures where it is natural to view objects as nodes and pointers as edges between the object storing the pointer and the object pointed to.

When humans think about graphs, they usually find it convenient to work with pictures showing nodes as bullets and edges as lines and arrows. For treating graphs algorithmically, a more mathematical notation is needed: A *directed graph* $G = (V, E)$ is a pair consisting of a *node set* (or *vertex* set) V and an *edge set* $E \subseteq V \times V$. We sometimes abreviate directed graph to *digraph*. For example, Figure 2.7 shows the graph $G = (\{s, t, u, v, w, x, y, z\}, \{(s, t), (t, u), (u, v), (v, w), (w, x), (x, y), (y, z), (z, s), (s, v), (z, w), (y, t), (x, u)\})$. Throughout this book, we use the convention $n = |V|$ and $m = |E|$ if no other definitions for n or m are given. An edge $e = (u, v) \in E$ represents a connection from u to v. We call u and v the *source* and *target* of e, respectively. We say that e is *incident* to u and v and that v and u are *adjacent*. The special case of a *self-loop* (v, v) is disallowed unless specifically mentioned.

The *outdegree* of a node v is the number of edges leaving it and its *indegree* is the number of edges ending at it, formally, $\mathit{outdegree}(v) = |\{(v, u) \in E\}|$ and $\mathit{indegree}(v) = |\{(u, v) \in E\}|$. For example, node w in graph G in Figure 2.7 has indegree two and outdegree one.

A *bidirected graph* is a digraph where for any edge (u, v) also the reverse edge (v, u) is present. An *undirected graph* can be viewed as a streamlined representation of a bidirected graph where we write a pair of edges (u, v), (v, u) as the two element set $\{u, v\}$. Figure 2.7 shows a three node undirected graph and its bidirected counterpart. Most graph theoretic terms for undirected graphs have the same definition as for their bidirected counterparts so that this section concentrates on directed graphs and only mentions undirected graphs when there is something special about them. For example, the number of edges of an undirected graph is only half the number of edges of its bidirected counterpart. Nodes of an undirected graph have identical in- and outdegree and so we simply talk about their *degree*. Undirected graphs are important because directions often do not matter and because many problems are easier to solve (or even to define) for undirected graphs than for general digraphs.

A graph $G' = (V', E')$ is a *subgraph* of G if $V' \subseteq V$ and $E' \subseteq E$. Given $G = (V, E)$ and a subset $V' \subseteq V$, the subgraph *induced* by V' is defined as $G' = (V', E \cap (V' \times V'))$. In Figure 2.7, the node set $\{v, w\}$ in G induces the subgraph $H = (\{v, w\}, \{(v, w)\})$. A subset $E' \subseteq E$ of edges induces the subgraph (V, E').

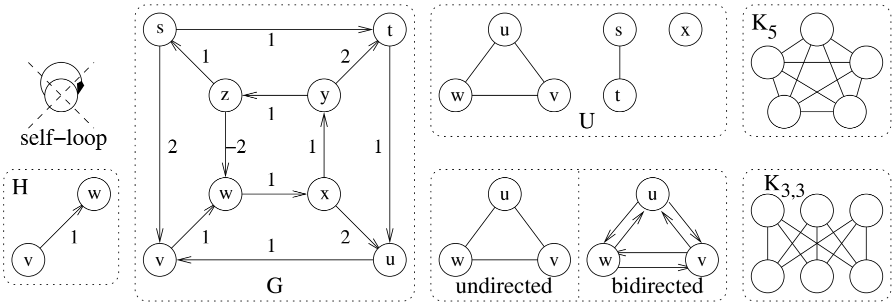


Fig. 2.7. Some graphs.

Often additional information is associated with nodes or edges. In particular, we will often need *edge weights* or *costs* $c : E \to \mathbb{R}$ mapping edges to some numeric value. For example, the edge (z, w) in graph G from Figure 2.7 has weight $c((z, w)) = -2$. Note that edge $\{u, v\}$ of an undirected graph has a unique edge weight whereas in a bidirected graph we can have $c((u, v)) \neq c((v, u))$.

We have now seen quite a lot of definitions on one page of text. If you want to see them at work, you may want to jump to Chapter 8 to see algorithms operating on graphs. But things are also becoming more interesting here.

An important higher level graph-theoretic concept is the notion of a path. A *path* $p = \langle v_0, \ldots, v_k \rangle$ is a sequence of nodes in which subsequent nodes are connected by edges in E, i.e, $(v_0, v_1) \in E$, $(v_1, v_2) \in E$, $\ldots$, $(v_{k-1}, v_k) \in E$; p has length k and runs from v_0 to v_k. Sometimes a path is also represented by its sequence of edges. For example, $\langle u, v, w \rangle = \langle (u, v), (v, w) \rangle$ is a path of length two in Figure 2.7. A path is *simple* if its nodes, except maybe for v_0 and v_k, are pairwise distinct. In Figure 2.7, $\langle z, w, x, u, v, w, x, y \rangle$ is a non-simple path.

Cycles are paths with a common first and last node. A simple cycle visiting all nodes of a graph is called a *Hamiltonian* cycle. $\langle s, t, u, v, w, x, y, z, s \rangle$ in graph G in Figure 2.7 is Hamiltonian. A simple undirected cycle contains at least three nodes since we also do not allow edges to be used twice in simple undirected cycles.

The concept of paths and cycles helps us to define yet higher level concepts. A digraph is *strongly connected*, if for any two nodes u and v there is a path from u to v. Graph G in Figure 2.7 is strongly connected. A strongly connected component of a digraph is a maximal node-induced strongly connected subgraph. Removing edge (w, x) from G in Figure 2.7, we obtain a digraph without any directed cycles. A digraph without any cycles is called a *directed acyclic graph (DAG)*. In a DAG, every strongly connected component consists of a single node. An undirected graph is *connected* if the corresponding bidirected graph is strongly connected. The connected components are the strongly connected components of the corresponding bidirected graph. For example, graph U in Figure 2.7 has connected components $\{u, v, w\}$, $\{s, t\}$, and $\{x\}$. Node set $\{u, w\}$ induces a connected subgraph but it is not maximal and hence not a component.

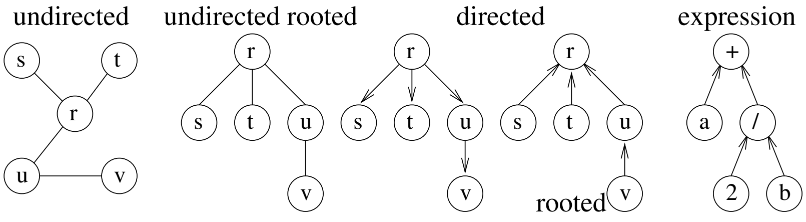


Fig. 2.8. Different kinds of trees: From left to right, we see an undirected tree, an undirected rooted tree, a directed out-tree, a directed in-tree, and an arithmetic expression.

An undirected graph is a *tree* if there is *exactly* one path between any pair of nodes; see Figure 2.8 for an example. An undirected graph is a *forest* if there is *at most* one path between any pair of nodes. Note that each component of a forest is a tree.

Lemma 8. *The following properties of an undirected graph G are equivalent:*

1. *G is a tree.*
2. *G is connected and has exactly $n - 1$ edges.*
3. *G is connected and contains no cycles.*

Proof. In a tree, there is a unique path between any two nodes. Hence the graph is connected and contains no cycles. Conversely, if there are two nodes that are connected by more than one path, the graph contains a cycle. Thus (1) and (3) are equivalent. We next show the equivalence of (2) and (3). So assume that $G = (V, E)$ is connected and let $m = |E|$. Perform the following experiment. Start with the empty graph and add the edges in E one by one. Addition of an edge can reduce the number of connected components by at most one. We start with n components and must end up with one component. Thus $m \geq n - 1$. Assume now that there is an edge $e = \{u, v\}$ whose addition does not reduce the number of connected components. Then u and v are already connected by a path and hence addition of e creates a cycle. If G is cycle-free, this case cannot occur and hence $m = n - 1$. Thus (3) implies (2). Assume next that G is connected and has exactly $n - 1$ edges. Again add the edges one by one and assume that adding $e = \{u, v\}$ creates a cycle. Then u and v are already connected and hence e does not reduce the number of connected components. Thus (2) implies (3).

Lemma 8 does not carry over to digraphs. For example, a DAG may have many more than $n - 1$ edges. A directed graph is an *out-tree* with *root* node r if there is exactly one path from r to any other node. It is an *in-tree* with root node r if there is exactly one path from any other node to r. Figure 2.8 shows examples.

We can also make an undirected graph rooted by declaring one of its nodes as the root. Computer scientists have the peculiar habit to draw rooted trees with the root at the top and all edges going downward. For rooted trees, it is customary to denote relations between nodes by terms borrowed from family relations. Edges go between a unique *parent* and its *children*. Nodes with the same parent are *siblings*. Nodes without childred are *leaves*. Non-root, non-leaf nodes are *interior* nodes. Consider a path such that u is between the root and another node v. Then u is an *ancestor* of v and v is a *descendant* of u. A node u and its descendants form a *subtree* rooted at u. For example, in Figure 2.8 r is the root; s, t, and v are leaves; s, t, and u are siblings because they are children of the same parent r; v is an interior node; r and u are ancestors of v; s, t, u and v are descendants of r; v and u form a subtree rooted at u.

It is time for a graph algorithm. We will describe an algorithm for testing whether a directed graph is acyclic. We use the simple observation that a node v with outdegree zero cannot appear in any cycle. Hence, by deleting v (and its incoming edges) from the graph, we obtain a new graph G' that is acyclic if and only if G is acyclic. By iterating this transformation, we either arrive at the empty graph which is certainly acyclic, or we obtain a graph G^* where every node has outdegree at least one. In the latter case, it is easy to find a cycle: Start at any node v and construct a path by repeatedly choosing an arbitrary outgoing edge until you reach a node v' that you have seen before. The constructed path will have the form $(v, \ldots, v', \ldots, v')$, i.e., the part $(v', \ldots, v')$ forms a cycle. For example, in Figure 2.7 graph G has no node with outdegree zero. To find a cycle, we might start at node z and follow the walk $\langle z, w, x, u, v, w \rangle$ until we encounter w a second time. Hence, we have identified the cycle $\langle w, x, u, v, w \rangle$. In contrast, if edge (w, x) is removed, there is no cycle. Indeed, our algorithm will remove all nodes in the order w, v, u, t, s, z, y, x. In Chapter 8 we will see how to represent graphs such that this algorithm can be implemented to run in linear time. See also Exercise 151. We can easily make our algorithm certifying. If the algorithm finds a cycle, the graph is certainly cyclic. If the algorithm reduces the graph to the empty graph, number the nodes in increasing order in which they are removed from G. Since we always remove a node v of outdegree zero in the current graph, any edge out of v in the original graph must go a node that was removed previously and hence has received a smaller number. Thus the ordering proves acyclicity: along any edge, the node numbers decrease.

Ordered Trees: Trees are ideally suited to represent hierarchies. For example, consider the expression $a + 2/b$. We have learned that this expression means that a and $2/b$ are added. But deriving this from the sequence of characters $\langle a, +, 2, /, b \rangle$ is difficult. For example, it requires knowledge of the rule that division binds more tightly than addition. Therefore compilers isolate this syntactical knowledge in so-called *parsers* that produce a more structured representation based on trees. Our example would be transformed into the expression tree given in Figure 2.8. Such trees are directed and in contrast to graph theoretic trees, they are *ordered*. In our example, a is the first or left child of the root and / is the right or second child of the root.

Expression trees are easy to evaluate by a simple recursive algorithm. Figure 2.9 shows an algorithm for evaluating expression trees whose leaves are numbers and whose interior nodes are binary operators (say +,-,*,/).

```
**Function** *eval*$(r)$ : $\mathbb{R}$
    **if** $r$ *is a leaf* **then return** *the number stored in* $r$
    **else**                                              // $r$ is an operator node
        $v_1$:=*eval*(*first child of* $r$)
        $v_2$:=*eval*(*second child of* $r$)
        **return** $v_1$ *operator*$(r)v_2$                   // apply the operator stored in $r$
```

Fig. 2.9. Recursive evaluation of an expression tree rooted at r.

We will see many more examples of ordered trees in this book. Chapters 6 and 7 use them to represent fundamental data structures and Chapter 12 uses them to systematically explore solution spaces.

Exercise 24. Describe ten substantially different applications that can be modeled using graphs; car and bicycle networks are not considered substantially different. At least five should not be mentioned in this book.

Exercise 25. Exhibit an n node DAG that has $n(n-1)/2$ edges.

Exercise 26. A *planar graph* is a graph that can be drawn on a sheet of paper such that no two edges cross each other. Argue street networks are *not* necessarily planar. Show that the graphs K_5 and K_{33} in Figure 2.7 are not planar.

2.10 P and NP

When should we call an algorithm efficient? Are there problems for which there is no efficient algorithm? Of course, drawing the line between "efficient" and "inefficient" is a somewhat arbitrary business. But as a first approximation, the following distinction has proved useful: An algorithm $\mathcal{A}$ runs in *polynomial time* or is a *polynomial time algorithm* if there is a polynomial $p(n)$ such that its execution time on inputs of size n is $\mathcal{O}(p(n))$. If not otherwise mentioned, the size of the input will be measured in bits. A problem can be solved in *polynomial time* if there is a polynomial time algorithm solving it. We equate efficiently solvable with polynomial time solvable. All chapters of this book except for Chapter 12 are about efficient algorithms. A big advantage of this definition is that implementation details are usually not important. For example, it does not matter whether a clever data structure can accelerate an $\mathcal{O}(n^3)$ algorithm by a factor n.

There are many problems for which no efficient algorithm is known. Here are six:

Hamiltonian Cycle Problem: given an undirected graph, decide whether it contains a Hamiltonian cycle.

Boolean Satisfiability Problem: given a boolean expression in conjunctive form, decide whether it has a satisfying assignment. A boolean expression in conjunctive form is a conjunction $C_1 \wedge C_2 \wedge \ldots \wedge C_k$ of clauses. A clause is a disjuntion

$\ell_1 \vee \ell_2 \vee \ldots \vee \ell_h$ of literals and a literal is a variable or a negated variable. So $v_1 \vee \neg v_3 \vee \neg v_9$ is a clause.

Clique Problem: Given an undirected graph and an integer k, decide whether the graph contains a complete subgraph (= a clique) on k nodes.

Knapsack Problem: Given n pairs of integers (w_i, p_i) and integers M and P, decide whether there is a subset $I \subseteq [1..n]$ such that $\sum_{i \in I} w_i \leq M$ and $\sum_{i \in I} p_i \geq P$.

Traveling Salesman Problem: Given an edge-weighted undirected graph and an integer C, decide whether the graph contains a Hamiltonian cycle of length at most C.

Graph Coloring: Given an undirected graph and an integer k, decide whether there is a coloring of the nodes with k colors such that any two adjacent nodes are colored differently.

The fact that we know no efficient algorithms for these problems, does not imply that none exist. It is simply not known, whether an efficient algorithm exists or not. In particular, we have no proof that they do not exist. In general, it is very hard to prove that a problem cannot be solved in a given time bound. We will see some simple lower bounds in Section **??**. Most algorithmicists believe that the three problems above have no efficient algorithm.

Complexity theory has found an interesting surrogate for the absence of lower bound proofs. It clusters algorithmic problems into large groups that are equivalent with respect to some complexity measure. In particular, there is a large class of equivalent problems known as $\mathbf{NP}$-*complete* problems. Here, $\mathbf{NP}$ is an abbreviation for non-deterministic polynomial time. If the term non-deterministic polynomial time does not mean anything to you, ignore it and carry on. The three problems mentioned above are $\mathbf{NP}$-complete and so are many other natural problems. It is widely believed that $\mathbf{P}$ is a proper subset of $\mathbf{NP}$. This would imply, in particular, that $\mathbf{NP}$-complete problems have no efficient algorithm. In the remainder of this section, we will give a formal definition of the class $\mathbf{NP}$. We refer the reader to books about theory of computation and complexity theory [72, 12, 169, 192] for a thorough treatment.

We assume, as in customary in complexity theory, that inputs are encoded in some fixed finite alphabet Σ. A *decision problem* is a subset $L \subseteq \Sigma^*$. We use χ_L to denote the characteristic function of L, i.e, $\chi_L(x) = 1$ if $x \in L$ and $\chi_L(x) = 0$ if $x \notin L$. A decision problem is polynomial time solvable iff its characteristic function is polynomial time computable. We use $\mathbf{P}$ to denote the class of polynomial time solvable decision problems.

A decision problem L is in $\mathbf{NP}$ iff there is a predicate $Q(x, y)$ and a polynomial p such that

1. for any $x \in \Sigma^*$: $x \in L$ iff there is a $y \in \Sigma^*$ with $|y| \leq p(|x|)$ and $Q(x, y)$ and
2. Q is computable in polynomial time.

We call y a *witness* or *proof* of membership. For our three example problems, it is easy to show that they belong to $\mathbf{NP}$. In case of the Hamiltonian cycle problem, the witness is a Hamiltonian cycle in the input graph, in the Boolean satisfiablity problem, the witness is a satisfying assignment, and in the clique problem, the witness is a clique of size k.

A decision problem L is *polynomial time reducible* (or simply *reducible*) to a decision problem L' if there is a polynomial time computable function g such that for all $x \in \Sigma^*$, we have $x \in L$ iff $g(x) \in L'$. Clearly, if L is reducible to L' and $L' \in \mathbf{P}$ then $L \in \mathbf{P}$. Also, reducibility is transitive. A decision problem L is $\mathbf{NP}$*-hard* if every problem in $\mathbf{NP}$ is polynomial time reducible to it. A problem is $\mathbf{NP}$*-complete* if it is an $\mathbf{NP}$-hard and in $\mathbf{NP}$. At first glance, it seems prohibitively difficult to prove any problem $\mathbf{NP}$-complete — one would have to show that *every* problem in $\mathbf{NP}$ is polynomial time reducible to it. However, in 1971, Cook and Levin independently managed to do this for the boolean satisfiability problem [45, 116]. From then on it was "easy". Assume you want to show that problem L is $\mathbf{NP}$-complete. You need to show two things: (1) $L \in \mathbf{NP}$ and (2) there is *some* known $\mathbf{NP}$-complete problem L' that can be reduced to it. Transitivity of the reducibility relation then implies that all problems in $\mathbf{NP}$ are reducible to L. With every new complete problem, it becomes simpler to show that other problems are $\mathbf{NP}$-complete. The website `http://www.nada.kth.se/~viggo/wwwcompendium/wwwcompendium.html` maintains a compendium of $\mathbf{NP}$-complete problems. We give one example for a reduction.

Lemma 9. *The boolean satisfiability problem is polynomial time reducible to the clique problem.*

Proof. Let $F = C_1 \wedge \ldots \wedge C_k$ with $C_i = \ell_{i1} \vee \ldots \vee \ell_{ih_i}$ and $\ell_{ij} = x_{ij}^{\beta_{ij}}$ be a formula in conjunctive form. Here x_{ij} is a variable and $\beta_{ij} \in \{0,1\}$. A superscript 0 indicates a negated variable. Consider the following graph G. Its vertices V represent the literals in our formula, i.e., $V = \{r_{ij} : 1 \le i \le k \text{ and } 1 \le j \le h_i\}$. Two vertices r_{ij} and $r_{i'j'}$ are connected by an edge iff $i \ne i'$ and either $x_{ij} \ne x_{i'j'}$ or $\beta_{ij} = \beta_{i'j'}$. In words, the representatives of two literals are connected by an edge if they belong to different clauses and an assignment can satisfy them simultaneously. We claim that F is satisfiable iff G has a clique of size k.

Assume first that there is a satisfying assignment α. The assignment must satisfy at least one literal in every clause, say literal ℓ_{ij_i} in clause C_i. Consider the subgraph of G spanned by the r_{ij_i}, $1 \le i \le k$. It is a clique of size k. Assume otherwise, say r_{ij_i} and $r_{i'j_{i'}}$ are not connected by an edge. Then $x_{ij_i} = x_{i'j_{i'}}$ and $\beta_{ij_i} \ne \beta_{i'j_{i'}}$. But then literals ℓ_{ij_i} and $\ell_{i'j_{i'}}$ are complements of each other and α cannot satisfy them both.

Conversely, assume that there is a clique K of size k in G. We construct a satisfying assignment α. For each i, $1 \le i \le k$, K contains exactly one vertex r_{ij_i}. We construct a satisfying assignment α by setting $\alpha(x_{ij_i}) = \beta_{ij_i}$. Note that α is well-defined because $x_{ij_i} = x_{i'j_{i'}}$ implies $\beta_{ij_i} = \beta_{i'j_{i'}}$; otherwise r_{ij_i} and $r_{i'j_{i'}}$ would not be connected by an edge. α clearly satisfies F.

Exercise 27. Show that the Hamiltonian cycle problem is polynomial time reducible to the Traveling Salesman problem.

All $\mathbf{NP}$-complete problems have a common destiny. If anybody finds a polynomial time algorithm for *one* of them, $\mathbf{NP}$ and $\mathbf{P}$ collapse. Since so many people have tried to find such solutions, it becomes less and less likely that this will ever happen: the $\mathbf{NP}$-complete problems are mutual witnesses of their hardness.

Does the theory of $\mathbf{NP}$-completeness also apply to optimization problems? Optimization problems are easy turned into decision problems. Instead of asking for an optimal solution we ask the question whether there is a solution with objective value greater or equal to k where k is an additional input. Conversely, if we have an algorithm to decide whether there is a solution with value greater or equal to k, we can use exponential and binary search (see Section 2.5) to find the optimal objective value.

An algorithm for a decision problem returns yes or no depending on whether the instance belongs to the problem or not. It does not return a witness. Frequently, witnesses can be constructed by applying the decision algorithm repeatedly. Assume we want to find a clique of size k, but have only an algorithm that decides whether a clique of size k exists. We select an arbitrary node v and ask whether $G' = G \setminus v$ has a clique of size k. If so, we recursively search for a clique in G'. If not, we know that v must be part of the clique. Let V' be the set of neighbors of v. We recursively search for a clique C_{k-1} of size $k-1$ in the subgraph spanned by V'. Then $v \cup C_{k-1}$ is a clique of size k in G.

2.11 Implementation Notes

Our pseudocode is easily converted into actual programs in any imperative programming language. We will give more detailed comments for C++ and Java below. The Eiffel programming language [132] has extensive support for assertions, invariants, preconditions, and postconditions.

Our special values $\perp$, $-\infty$, and ∞ are available for floating point numbers. For other data types, we have to emulate these values. For example, one could use the smallest and largest representable integers for $-\infty$, and ∞ respectively. Undefined pointers are often represented as a null pointer **null** . Sometimes we use special values for convenience only and a robust implementation should circumvent using them. You will find examples in later chapter.

Randomized algorithms need access to a random source. You have the choice between a hardware generator that generates true random numbers or an algorithmic generator that generates pseudo-random numbers. We refer the reader to the Wikipedia page on random numbers for more information.

C++: Our pseudocode can be viewed as a concise notation for a subset of C++. The memory management operations **allocate** and **dispose** are similar to the C++ operations `new` and `delete`. C++ calls the default constructor for each element of an array, i.e., allocating an array of n objects takes time $\Omega(n)$ whereas allocating an array n of `int`s takes constant time. In contrast, we assume that *all* arrays which are not explicitly initialized contain garbage. In C++ you can obtain this effect using the C functions `malloc` and `free`. However, this is a deprecated practice and should only be used when array initialization would be a severe performance bottleneck. If memory management of many small objects is performance critical, you can customize it using the `allocator` class of the C++ standard library.

Our parameterization of classes using **of** is a special case of the C++-template mechanism. The parameters added in brackets after a class name correspond to the parameters of a C++ constructor.

Assertions are implemented as C-macros in the include file `assert.h`. By default, violated assertions trigger a runtime error and print the line number and file where the assertion was violated. If the macro `NDEBUG` is defined, assertion checking is disabled.

For many data structures and algorithms discussed in this book, excellent implementations are available in software libraries. Good sources are the standard template library STL [148], the Boost [28] C++ libraries, and the LEDA [115] library of efficient algorithms and data structures.

Java: Java has no explicit memory management. Rather, a *garbage collector* periodically recycles pieces of memory that are no longer referenced. While this simplifies programming enormously, it can be a performance problem. Remedies are beyond the scope of this book. Generic types provide parameterization of classes. Assertions are implemented with the `assert` statement.

Excellent implementations for many data structures and algorithms are available in the package `java.util` and in the JDSL [77] data structure library in Java.

2.12 Historical Notes and Further Findings

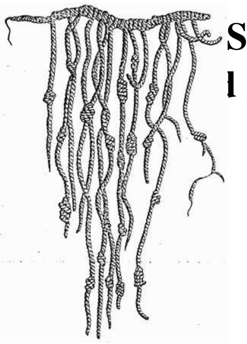
Sheperdson and Sturgis [168] defined the RAM-model for use in algorithmic analysis. The RAM model restricts cells to hold a logarithmic number of bits. Dropping this assumption has undesirable consequences, e.g., the complexity classes $\mathbf{P}$ and $\mathbf{PSPACE}$ collapse [86]. Knuth [110] describes a more detailed abstract machine model.

Floyd [62] introduced the method of invariants to assign meaning to programs and Hoare [90, 91] systemized their use.

The book [80] is a compendium on sums and recurrences and, more generally, discrete mathematics.

Books on compiler construction [137, 194] tell you more about the compilation of high-level programming languages into machine code.

3



Sequences
l Linked Lists

[todo: Titel im Inhaltsverzeichnis reparieren] ⇐

[todo: Bilder positionieren] *Perhaps the world's oldest data structures were tablets in cuneiform script used more than 5000 years ago by custodians in Sumerian temples. They kept lists of goods, their quantities, owners and buyers. The picture on the left shows an example. Possibly this was the first application of written language. The operations performed on such lists have remained the same — adding entries, storing them for later, searching entries and changing them, going through a list to compile summaries, etc. The Peruvian quipu you see in the picture on the right served a similar purpose in the Inca empire using knots in colored strings arranged sequentially on a master string. Probably it is easier to maintain and use data on tablets than using knotted string, but one would not want to haul stone tablets over the Andean mountain trails. Apparently, it makes sense to consider different representations for the same kind of logical data.* ⇐

The abstract notion of a sequence, list, or table is very simple and is independent of its representation in a computer. Mathematically, the only important property is that the elements of a sequence $s = \langle e_0, \ldots, e_{n-1} \rangle$ are arranged in a linear order — in contrast to the trees and graphs in Chapters 7 and 8, or the unordered hash tables discussed in Chapter 4. There are two basic ways for referring to the elements of a sequence.

One is to specify the index of an element. This is the way we usually think about arrays where $s[i]$ returns the i-th element of sequence s. Our pseudocode supports *static* arrays. In a *static* data structure, the size is known in advance and the data structure is not modified by insertions and deletions. In a *bounded* data structure, the maximal size is known in advance. In Section 3.2 we introduce *dynamic* or *unbounded arrays* that can grow and shrink as elements are inserted and removed. The analysis of unbounded arrays introduces the concept of *amortized analysis*.

The second way for referring to the elements of a sequence is relative to other elements. For example, one could ask for the successor of an element e, for the predecessor of an element e' or for the subsequence $\langle e, \ldots, e' \rangle$ of elements between e and e'. Although relative access can be simulated using array indexing, we will see in Section 3.1 that list-based representation of sequences is more flexible. In particular, it becomes easier to insert or remove arbitrary pieces of a sequence.

In many algorithms, it does not matter very much whether sequences are implemented using arrays or linked lists because only a very limited set of operations is needed that can be handled efficiently using either representation. Section 3.4 introduces stacks and queues which are the most common data types of that kind. In Section 3.5 we summarize the findings of the Chapter.

3.1 Linked Lists

In this section we study the representation of sequences by linked lists. In a doubly linked list each item points to its successor and to its predecessor. In a singly linked list each item points to its successor. We will see that linked lists are easily modified in many ways: we may insert or delete items or sublists, we may concatenate lists. The drawback is that random access (operator $[\cdot]$) is not supported. We study doubly linked lists in Section 3.1.1 and singly linked lists in Section 3.1.2. Singly linked lists are more space efficient and somewhat faster and should therefore be preferred whenever their functionality suffices. A good way to think of a linked list is to imagine a chain where one element is written on each link. Once we get hold of one link of the chain, we can retrieve all elements. [replace figure chain.ps ⟹ by http://de.fotolia.com/id/3797184?]

3.1.1 Doubly Linked Lists

Figure 3.1 shows the basic building block of a linked list. A list *item* stores an element and pointers to successor and predecessor. We call a pointer to a list item a *handle*. This sounds simple enough, but pointers are so powerful that we can make a big mess if we are not careful. What makes a consistent list data structure? We require that for each item it, the successor of the predecessor is equal to it and the predecessor of the successor is equal to it.

A sequence of n elements is represented by a ring of $n + 1$ items. There is a special or dummy item h which stores no element. The successor h_1 of h stores the first element of the sequence, the successor of h_1 stores the second element of the sequence, and so on. The predecessor of h stores the last element of the sequence,

```
Class Handle = Pointer to Item

Class Item of Element                          // one link in a doubly linked list
    e : Element
    next : Handle                              //
    prev : Handle
    invariant next→prev = prev→next = this
```

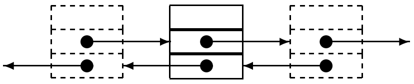


Fig. 3.1. The items of a doubly linked list.

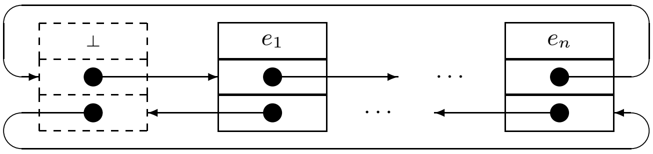


Fig. 3.2. The representation of sequence $\langle e_1, \ldots, e_n \rangle$ by a doubly linked list. There are $n + 1$ items arranged in a ring, a special item h containing no element and one item for each element of the sequence. The item containing e_i is the successor of the item containing e_{i-1} and the predecessor of the item containing e_{i+1}. The special item is between the item containing e_n and the item containing e_1.

see Figure 3.2. The empty sequence is represented by a ring consisting only of the special item. Since there are no elements in the sequence, the special item is its own successor and predecessor. Figure 3.4 contains the definition of the list representation of sequences. An object of class *List* contains a single list item h. The constructor of the class initializes the header h to an item containing $\perp$ and having itself as successor and predecessor. In this way, the list is initialized to the empty sequence.

We implement all basic list operations in terms of the single operation *splice* shown in Figure 3.3. *Splice* cuts out a sublist from one list and inserts it after some target item. The sublist is specified by handles a and b to its first and last element, respectively. In other words, b must be reachable from a by following zero or more next pointers and without going through the special element. The target item t can be either in the same list or in a different list; in the former case, it must not be inside the sublist starting at a and ending at b.

Splice does not change the number of items in the system. We assume that there is one special list, *freeList*, that keeps a supply of unused elements. When inserting new elements into a list, we take the necessary items from *freeList* and when deleting elements we return the corresponding items to *freeList*. The function *checkFreeList* allocates memory for new items when necessary. We defer its implementation to Exercise 30 and a short discussion in Section 3.6.

With these conventions in place, a large number of useful operations can be implemented as one line functions that all run in constant time. Thanks to the power of *splice*, we can even manipulate arbitrarily long sublists in constant time. Figures 3.4 and 3.5 show many examples. In order to test whether a list is empty, we simply

```
// Remove $\langle a,\ldots,b\rangle$ from its current list and insert it after $t$
// $\ldots,a',a,\ldots,b,b',\ldots + \ldots,t,t',\ldots \mapsto \ldots,a',b',\ldots + \ldots,t,a,\ldots,b,t',\ldots$

**Procedure** *splice*$(a,b,t : Handle)$
    **assert** *a and b belong to the same list, b is not before a, and* $t \notin \langle a,\ldots,b\rangle$
    // cut out $\langle a,\ldots,b\rangle$
    $a' := a \rightarrow prev$
    $b' := b \rightarrow next$
    $a' \rightarrow next := b'$
    $b' \rightarrow prev := a'$

    // insert $\langle a,\ldots,b\rangle$ after $t$
    $t' := t \rightarrow next$

    $b \rightarrow next := t'$
    $a \rightarrow prev := t$

    $t \rightarrow next := a$
    $t' \rightarrow prev := b$
```

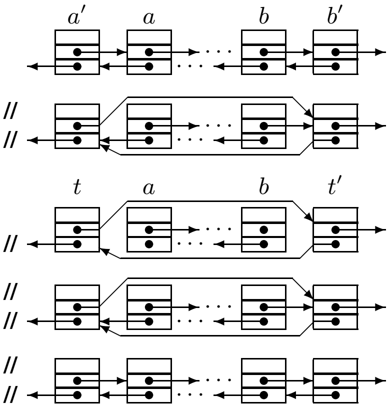


Fig. 3.3. Splicing lists.

```
**Class** *List* **of** *Element*
    // Item $h$ is the predecessor of the first element and the successor of the last element.
    $h = \begin{pmatrix} \perp \\ \texttt{this} \\ \texttt{this} \end{pmatrix}$ : *Item*                    // init to empty sequence
    // Simple access functions
    **Function** *head*() : *Handle;* **return address of** $h$          // Pos. before any proper element

    **Function** *isEmpty* : $\{0,1\}$; **return** *h.next* = **this**                    // $\langle\rangle$?
    **Function** *first* : *Handle;* **assert** $\neg$*isEmpty;* **return** *h.next*
    **Function** *last* : *Handle;* **assert** $\neg$*isEmpty;* **return** *h.prev*

    // Moving elements around within a sequence.
    // $(\langle\ldots,a,b,c\ldots,a',c',\ldots\rangle) \mapsto (\langle\ldots,a,c\ldots,a',b,c',\ldots\rangle)$
    **Procedure** *moveAfter(b, a' : Handle) splice*$(b,b,a')$
    **Procedure** *moveToFront*$(b : Handle)$ *moveAfter*$(b, head)$
    **Procedure** *moveToBack*$(b : Handle)$ *moveAfter*$(b, last)$
```

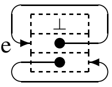


Fig. 3.4. Some constant time operations on doubly linked lists.

check whether h is its own successor. If a sequence is non-empty, its first and last element are the successor and predecessor of h, respectively. In order to move an item b after an item a', we simply cut out the sublist starting and ending at b and insert it after a'. This is exactly what $splice(b,b,a')$ does. In order to move an element to the first or last position of a sequence, we simply move it after head or after last. In order

```
// Deleting and inserting elements.
// $\langle \ldots, a, b, c, \ldots \rangle \mapsto \langle \ldots, a, c, \ldots \rangle$
Procedure remove($b$ : Handle) moveAfter(b, freeList.head)
Procedure popFront remove(first)
Procedure popBack remove(last)

// $\langle \ldots, a, b, \ldots \rangle \mapsto \langle \ldots, a, e, b, \ldots \rangle$
Function insertAfter(x : Element; a : Handle) : Handle
    checkFreeList              // make sure freeList is nonempty. See also Exercise 30
    $a' := freeList.first$                             // Obtain an item $a'$ to hold $x$,
    $moveAfter(a', a)$                                     // put it at the right place.
    $a' \to e := x$                                // and fill it with the right content.
    return $a'$

Function insertBefore(x : Element; b : Handle) : Handle return insertAfter(e, pred(b))
Procedure pushFront(x : Element) insertAfter(x, head)
Procedure pushBack(x : Element) insertAfter(x, last)

// Manipulations of entire lists
// $(\langle a, \ldots, b\rangle, \langle c, \ldots, d\rangle) \mapsto (\langle a, \ldots, b, c, \ldots, d\rangle, \langle\rangle)$
Procedure concat($L'$ : List)
    splice($L'$.first, $L'$.last, last)

// $\langle a, \ldots, b\rangle \mapsto \langle\rangle$
Procedure makeEmpty
    freeList.concat(this )
```

//

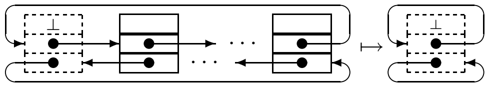


Fig. 3.5. More constant time operations on doubly linked lists.

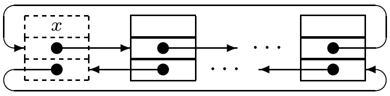
to delete an element b, we move it to *freeList*. To insert a new element e, we take the first item of *freeList*, store the element in it and move it to the place of insertion.

There are alternative ways of representing sequences by lists. A popular one avoids the special list item h and instead stores a handle to the first list item in the list object.

Exercise 28 (Alternative list implementation). Discuss an alternative implementation of *List* that does not need the dummy item h. Instead it stores a handle to the first list item in the list object. In the interfaces, the position before the first list element is encoded as a null pointer. The interface and the asymptotic execution times of all operations should remain the same. Give at least one advantage and one disadvantage of this implementation compared to the one given in the text.

The dummy item is also useful for other operations. For example, consider the problem of finding the next occurrence of an element x starting at item *from*. If x is not present, *head* should be returned. We use the dummy element as a *sentinel*. A sentinel is an element in a data structure that makes sure that some loop will terminate. In the case of lists, we store the key we are looking for in the dummy element. This ensures that x is present in the list structure and hence a search for it will always terminate. It will terminate in a proper list item or the dummy item depending on whether x is present in the list originally. The trick of using $head$ as a sentinal saves us an additional test in each iteration, namely, whether or not the end of the list is reached.

```
Function findNext($x$ : Element; from : Handle) : Handle
    $h.e = x$                           // Sentinel
    while $from \rightarrow e \neq x$ do
        $from := from \rightarrow next$
    return from
```



Exercise 29. Implement a procedure $swap$ that swaps two sublists in constant time, i.e., sequences $(\langle \ldots, a', a, \ldots, b, b', \ldots \rangle, \langle \ldots, c', c, \ldots, d, d', \ldots \rangle)$ are transformed into $(\langle \ldots, a', c, \ldots, d, b', \ldots \rangle, \langle \ldots, c', a, \ldots, b, d', \ldots \rangle)$. Is $splice$ a special case of $swap$?

Exercise 30 (Memory management for lists). Implement the function $checkFreelist$ called by $insertAfter$ in Figure 3.5. Since an individual call of the programming language primitive **allocate** for every single item might be too slow, your function should allocate space for items in large batches. The worst case execution time of $checkFreeList$ should be independent of the batch size. Hint: In addition to $freeList$ use a small array of free items.

Exercise 31. Give a constant time implementation for rotating a list to the right: $\langle a, \ldots, b, c \rangle \mapsto \langle c, a, \ldots, b \rangle$. Generalize your algorithm to rotate $\langle a, \ldots, b, c, \ldots, d \rangle$ to $\langle c, \ldots, d, a, \ldots, b \rangle$ in constant time.

Exercise 32. $findNext$ using sentinels is faster than an implementation that checks for the end of the list in each iteration. But how much faster? What speed difference do you predict for many searches in a small list with 100 elements, or for a large list with 10 000 000 elements respectively? Why is the relative speed difference dependent on the size of the list?

Maintaining the Size of a List

In our simple list data type, it is not possible to determine the number of elements in constant time. This can be fixed by introducing a member variable $size$ that is updated whenever the number of elements changes. Operations that affect several lists now need to know about the lists involved even if low level functions such as $splice$ would only need handles to the items involved. For example, consider the following code for moving an element a from a list L to the position after a' in list L':

```
Procedure moveAfter(b, $a'$ : Handle; L, $L'$ : List)
    splice(b,b,$a'$);    $L.size$−−;    $L'.size$++
```

Maintaining the size of lists interferes with other list operations. When we move elements as above, we need to know the sequences containing them and, more seriously, operations, that move around sublists between lists, cannot be implemented in constant time any more. The next exercise offers a compromise.

Exercise 33. Design a list data type that allows sublists to be moved between lists in constant time and allows constant time access to $size$ whenever sublist operations have not been used since the last access to the list size. When sublist operations have been used, $size$ is only recomputed when needed.

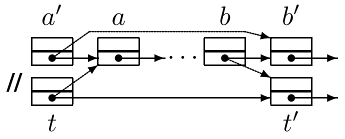
Exercise 34. Explain how the operations $remove$, $insertAfter$, and $concat$ have to be modified to keep track of the length of a $List$.

3.1.2 Singly Linked Lists

The two pointers per item of a doubly linked list make programming quite easy. Singly linked lists are the lean sisters of doubly linked lists. We use $SItem$ to refer to an item in a singly linked list. $SItem$s scrap the predecessor pointer and only store a pointer to the successor. This makes singly linked lists more space efficient and often faster than their doubly linked brothers. The downside is that some operations can no longer be performed in constant time or can no longer be supported in full generality. For example, we can remove an $SItem$ only if we know its predecessor.

We adopt the implementation approach from doubly linked lists. $SItem$s form collections of cycles and an $SList$ has a dummy $SItem$ h that precedes the first proper element and is the successor of the last proper element. Many operations of $List$s can still be performed if we slightly change the interface. For example, the following implementation of $splice$ needs the *predecessor* of the first element of the sublist to be moved.

```
// $(\langle \ldots, a', a, \ldots, b, b' \ldots \rangle, \langle \ldots, t, t', \ldots \rangle) \mapsto (\langle \ldots, a', b' \ldots \rangle, \langle \ldots, t, a, \ldots, b, t', \ldots \rangle)$
Procedure splice($a'$,$b$,$t$ : SHandle)
    $\begin{pmatrix} a' \to next \\ t \to next \\ b \to next \end{pmatrix} := \begin{pmatrix} b \to next \\ a' \to next \\ t \to next \end{pmatrix}$
```



Similarly, $findNext$ should not return the handle of the $SItem$ with the next hit but its *predecessor* so that it remains possible to remove the element found. Consequently, $findNext$ can only start searching at the item *after* the item given to it. A useful addition to $SList$ is a pointer to the last element because it allows us to support $pushBack$ in constant time.

Exercise 35. Implement classes $SHandle$, $SItem$, and $SList$ for singly linked lists in analogy to $Handle$, $Item$, and $List$. Show that the functions below can be implemented to run in constant time. Operations $head$, $first$, $last$, $isEmpty$, $popFront$, $pushFront$, $pushBack$, $insertAfter$, $concat$, and $makeEmpty$ should have the same interface as before. Operations *moveAfter*, *moveToFront*, *moveToBack*, *remove*, *popFront*, and *findNext* need different interfaces.

We will see several applications of singly linked lists in later chapters, for example in hash tables in Section 4.1 or for mergesort in Section 5.2. We may also use singly linked lists to implement free lists of memory managers — even for items of doubly linked lists.

3.2 Unbounded Arrays

Consider an array data structure that, besides the indexing operation $[\cdot]$, supports the following operations *pushBack*, *popBack*, and *size*.

$$\begin{aligned}\langle e_0,\ldots,e_n\rangle.\mathit{pushBack}(e) &= \langle e_0,\ldots,e_n,e\rangle\\ \langle e_0,\ldots,e_n\rangle.\mathit{popBack} &= \langle e_0,\ldots,e_{n-1}\rangle\\ \mathit{size}(\langle e_0,\ldots,e_{n-1}\rangle) &= n\end{aligned}$$

Why are unbounded arrays important? Because in many situations we do not know in advance how large an array should be. Here is a typical example: suppose you want to implement the Unix command `sort` for sorting the lines of a file. You decide to read the file into an array of lines, sort the array internally, and finally output the sorted array. With unbounded arrays this is easy. With bounded arrays, you would have to read the file twice: once to find the number of lines it contains and once to actually load it into the array.

We come to the implementation of unbounded arrays. We emulate an unbounded array u with n elements by a dynamically allocated bounded array b with w entries, where $w \geq n$. The first n entries of b are used to store the elements of u. The last $w-n$ entries of b are unused. As long as $w > n$, *pushBack* simply increments n and uses the first unused entry of b for the new element. When $w = n$, the next *pushBack* allocates a new bounded array b' that is a constant factor larger (say a factor two). To reestablish the invariant that u is stored in b, the content of b is copied to the new array so that the old b can be deallocated. Finally, the pointer defining b is redirected to the new array. Deleting the last element with *popBack* is even easier since there is no danger that b may become too small. However, we might waste a lot of space if we allow b to be much larger than needed. The wasted space can be kept small by shrinking b when n becomes too small. Figure 3.6 gives the complete pseudocode for an unbounded array class. Growing and shrinking is performed using the same utility procedure *reallocate*. Our implementation uses constants α and β with $\beta = 2$ and $\alpha = 4$. Whenever the current bounded array becomes too small, we replace it by an array of β times the old size. Whenever the size of the current array becomes α times as large as its used part, we replace it by an array of size βn. The choice of α and β will become clear later.

```
Class UArray of Element
   Constant $\beta = 2 : \mathbb{R}_+$                                   // growth factor
   Constant $\alpha = 4 : \mathbb{R}_+$                                  // worst case memory blowup
   $w = 1 : \mathbb{N}$                                                  // allocated size
   $n = 0 : \mathbb{N}$    // current size. invariant $n \le w < \alpha n$ or $n = 0$ and $w \le \beta$
                                                                          n            w
   $b$ : Array $[0..w-1]$ of Element                  // b → [$e_0$|···|$e_{n-1}$|    ¦ ··· ¦    ]

   Operator $[i : \mathbb{N}]$ : Element
      assert $0 \le i < n$
      return $b[i]$

   Function size : $\mathbb{N}$     return $n$

   Procedure pushBack($e$ : Element)                 // Example for $n = w = 4$:
      if $n = w$ then                                 // b → [0|1|2|3]
         reallocate($\beta n$)                         // b → [0|1|2|3|  ¦  ¦  ¦  ]
      $b[n] := e$                                     // b → [0|1|2|3|e ¦  ¦  ¦  ]
      $n$++                                           // b → [0|1|2|3|e|  ¦  ¦  ]

   Procedure popBack                                  // Example for $n = 5$, $w = 16$:
      assert $n > 0$                        // b → [0|1|2|3|4|  ¦  ¦  ¦  ¦  ¦  ¦  ¦  ¦  ¦  ¦  ]
      $n$−−                                 // b → [0|1|2|3|4 ¦  ¦  ¦  ¦  ¦  ¦  ¦  ¦  ¦  ¦  ]
      if $\alpha n \le w \wedge n > 0$ then           // reduce waste of space
         reallocate($\beta n$)                         // b → [0|1|2|3|  ¦  ¦  ¦  ]

   Procedure reallocate($w' : \mathbb{N}$)           // Example for $w = 4$, $w' = 8$:
      $w := w'$                                       // b → [0|1|2|3]
      $b'$ := allocate Array $[0..w-1]$ of Element    // b' → [  ¦  ¦  ¦  ¦  ¦  ¦  ¦  ]
      $(b'[0], \ldots, b'[n-1]) := (b[0], \ldots, b[n-1])$   // b' → [0¦1¦2¦3¦  ¦  ¦  ¦  ]
      dispose $b$                                     // b → [~~0¦1¦2¦3~~]
      $b := b'$                          // pointer assignment b → [0|1|2|3|  ¦  ¦  ¦  ]
```

Fig. 3.6. Unbounded arrays

Amortized Analysis of Unbounded Arrays

Our implementation of unbounded arrays follows the algorithm design principle "make the common case fast". Array access with $[\cdot]$ is as fast as for bounded arrays. Intuitively, $pushBack$ and $popBack$ should "usually" be fast — we just have to update n. However, some insertions and deletions incur a cost of $\Theta(n)$. We will show that such expensive operations are rare and that any sequence of m operations starting with an empty array can be executed in time $\mathcal{O}(m)$.

Lemma 10. *Consider an unbounded array u that is initially empty. Any sequence $\sigma = \langle \sigma_1, \ldots, \sigma_m \rangle$ of $pushBack$ or $popBack$ operations on u is executed in time $\mathcal{O}(m)$.*

Lemma 10 is a non-trivial statement. A small and innocent looking change to the program invalidates it.

Exercise 36. Your manager asks you to change the initialization of α to $\alpha = 2$. He argues that it is wasteful to shrink an array only when already three fourths of it are unused. He proposes to shrink it already when $n \leq w/2$. Convince him that this is a bad idea by giving a sequence of m $pushBack$ and $popBack$ operations that would need time $\Theta\big(m^2\big)$ if his proposal were implemented.

Lemma 10 makes a statement about the amortized cost of $pushBack$ and $popBack$ operations. Although single operations may be costly, the cost of a sequence of m operations is $\mathcal{O}(m)$. If we divide the total cost for the operations in σ by the number of operations, we get a constant. We say that the *amortized cost* of each operation is constant. Our usage of the term *amortized* is similar to its usage in everyday language, but it avoids a common pitfall. “I am going to cycle to work every day from now on and hence it is justified to buy a luxury bike. The cost per ride will be very small — the investment will amortize”. Does this kind of reasoning sound familiar to you? The bike is bought, it rains, and all good intentions are gone. The bike has not amortized. We will insist that a large expenditure is justified by savings in the past and not by expected savings in the future. Suppose your ultimate goal is to go to work in a luxury car. However, you are not going to buy it on your first day of work. Instead you walk and put a certain amount of money per day into a savings account. At some point, you will be able to buy a bicycle. You continue to put money away. At some point later, you will be able to buy a small car, and even later you can finally buy a luxury car. In this way every expenditure can be paid for by past savings and all expenditures amortize. Using the notion of amortized costs, we can reformulate Lemma 10 more elegantly. The increased elegance also allows better comparisons between data structures.

Corollary 1. *Unbounded arrays implement the operation $[\cdot]$ in worst case constant time and the operations $pushBack$ and $popBack$ in amortized constant time.*

To prove Lemma 10, we use the *bank account* or *potential* method. We associate an *account* or *potential* with our data structure and force every $pushBack$ and $popBack$ to put a certain amount into this account. Usually, we call our unit of currency *token*. The idea is that whenever a call of $reallocate$ occurs, the balance of the account is sufficiently high to pay for it. The details are as follows. A token can pay for a constant amount of work. For each call $reallocate(\beta n)$ we withdraw n tokens from the account. Observe, that the cost of the call is $\mathcal{O}(n)$ and hence covered by the value of the tokens. We charge two tokens to each call of $pushBack$ and one token to each call of $popBack$. We next show that these charges suffice to cover the withdrawals made by $reallocate$.

The first call of $\mathit{reallocate}$ occurs when there is one element already in the array and a new element is inserted. The element already in the array deposited two tokens in the account and this more than covers the one token withdrawn by $\mathit{reallocate}$. The new element provides its tokens for the next call of $\mathit{reallocate}$.

After a call of $\mathit{reallocate}$ we have an array of w elements: $w/2$ slots are occupied and $w/2$ are free. The next call of $\mathit{reallocate}$ occurs when either $n = w$ or $4n \leq w$. In the first case, at least $w/2$ elements were added to the array since the last call of $\mathit{reallocate}$ and each one of them deposited two tokens. So we have at least w tokens available and can cover the withdrawal made by the next call of $\mathit{reallocate}$. In the latter case, at least $w/2 - w/4 = w/4$ elements were deleted from the array since the last call of $\mathit{reallocate}$ and each one of them deposited one token. So we have at least $w/4$ tokens available. The call of $\mathit{reallocate}$ needs at most $w/4$ tokens and hence the cost of the call is covered. This completes the proof of Lemma 10.

Exercise 37. Redo the argument above for general values of α and β and charge $\beta/(\beta - 1)$ tokens to each call of $\mathit{pushBack}$ and $\beta/(\alpha - \beta)$ tokens to each call of $\mathit{popBack}$. Let n' such that $w = \beta n'$. Then, after a $\mathit{reallocate}$, n' elements are occupied and $(\beta - 1)n' = ((\beta - 1)/\beta)w$ are free. The next call of $\mathit{reallocate}$ occurs when either $n = w$ or $\alpha n \leq w$. Argue that in both cases there are enough tokens.

Amortized analysis is an extremely versatile tool and so we think it is worthwhile to know alternative proof methods. We give two variants of the proof above.

We charged two tokens to each $\mathit{pushBack}$ and one token to each $\mathit{popBack}$. Alternatively, we could charge three tokens to each $\mathit{pushBack}$ and not charge $\mathit{popBack}$ at all. The accounting is simple. The first two tokens pay for the insertion as above and the third token is used when the element is deleted.

Exercise 38 (continuation of Exercise 37). Show that a charge of $\beta/(\beta - 1) + \beta/(\alpha - \beta)$ tokens to each $\mathit{pushBack}$ is enough. Determine values of α such that $\beta/(\alpha - \beta) \leq 1/(\beta - 1)$ and $\beta/(\alpha - \beta) \leq \beta/(\beta - 1)$, respectively.

We come to a second modification of the proof. In the argument above, we used a global argument in order to show that there are enough tokens in the account before each call of $\mathit{reallocate}$. We now show how to replace the global argument by a local argument. Recall that immediately after a call of $\mathit{reallocate}$ we have an array of w elements out of which $w/2$ are filled and $w/2$ are free. We now argue that at any time after the first call of $\mathit{reallocate}$ the following token invariant holds: the account contains at least $\max(2(n - w/2), w/2 - n)$ tokens. Observe that this number is always non-negative. We use induction on the number of operations. Immediately, after the first $\mathit{reallocate}$ there is one token in the account and the invariant requires none. A $\mathit{pushBack}$ increases n by one and adds 2 tokens. So the invariant is maintained. A $\mathit{popBack}$ removes one element and adds one token. So the invariant is maintained. When a call of $\mathit{reallocate}$ occurs, we have either $n = w$ or $4n \leq w$. In the former case, the account contains at least n tokens and n tokens are required for the reallocation. In the latter case, the account contains at least $w/4$ tokens and n are required. So in either case the number of tokens suffices.

Exercise 39. Charge three tokens to a $pushBack$ and no token to a $popBack$. Argue that the account contains always at least $n+\max(2(n-w/2), w/2-n) = \max(3n-w, w/2)$ tokens.

Exercise 40 (Popping many elements). Implement an operation $popBack(k)$ that removes the last k elements in amortized constant time independent of k.

Exercise 41 (Worst case constant access time). Suppose for a real time application you need an unbounded array data structure with *worst case* constant execution time for all operations. Design such a data structure. Hint: store the elements in up to two arrays. Start moving elements to a larger array well before the small array is completely exhausted.

Exercise 42 (Implicitly growing arrays). Implement unbounded arrays where the operation $[i]$ allows any positive index. When $i \geq n$, the array is implicitly grown to size $n = i + 1$. When $n \geq w$, the array is reallocated as for $UArray$. Initialize entries that have never been written with some default value $\perp$.

Exercise 43 (Sparse arrays). Implement bounded array with constant time for allocating arrays and constant time for operation $[\cdot]$. All array elements should be (implicitly) initialized to $\perp$. You are not allowed to make any assumptions on the contents of a freshly allocated array. Hint: Use an extra array of the same size and store the number t of array elements to which a value was already assigned. Then $t = 0$ initially. An array entry i to which a value was already assigned stores the value and an index j, $1 \leq j \leq t$, of the extra array and i is stored in that index of the extra array.

We give a second example of an amortized analysis, the amortized cost of incrementing a binary counter. The value n of the counter is represented by a sequence $\ldots\beta_i\ldots\beta_1\beta_0$ of binary digits, i.e., $\beta_i \in \{0,1\}$ and $n = \sum_{i\geq 0}\beta_i 2^i$. The initial value is zero. Its representation is a string of all zeroes. We define the cost of incrementing the counter as one plus the number of trailing ones in the binary representation, i.e., the transition

$$\ldots 01^k \rightarrow \ldots 10^k \quad \text{has cost } k+1.$$

What is the total cost of m increments? We show that the cost is $\mathcal{O}(m)$. Again, we give a global argument first and then a local argument.

When the counter is incremented m times, the final value is m. The representation of the number m requires $L = 1 + \lceil \log m \rceil$ bits. Among the numbers 0 to $m-1$ there are at most 2^{L-k-1} numbers whose binary representation ends with a zero followed by k ones. For each one of them the increment costs $1+k$. Thus the total cost of the m increments is bounded by

$$\sum_{0\leq k<L}(k+1)2^{L-k-1} = 2^L \sum_{1\leq k\leq L} k/2^k \leq 2^L \sum_{k\geq 1} k/2^k = 2\cdot 2^L \leq 4m\ .$$

Thus the amortized cost of an increment is $\mathcal{O}(1)$.

The argument above is global in the sense that it requires an estimate of the number of representations ending in a zero followed by k ones. We now give a local argument which does not need such a bound. We associate a bank account with the counter. Its balance is the number of ones in the binary representation of the counter. So the balance is initially zero. Consider an increment of cost $k+1$. Before the increment the representation ends in a zero followed by k ones, after the increment the representation ends in a one followed by $k-1$ zeroes. So the number of ones in the representation decreases by $k-1$, i.e., the operation releases $k-1$ tokens from the account. The cost of the increment is $k+1$. We cover $k-1$ tokens from the account and charge two tokens to the operation. Thus the total cost of m operations is at most $2m$.

3.3 Amortized Analysis

We give a general definition of amortized time bounds and amortized analysis. We recommend to read this section quickly and to come back to it when needed. We consider an arbitrary data structure. The values of all program variables comprise the state of the data structure; we use S to denote the set of states. In the example of the previous section, the state of our data structures is formed by the values of n, w, and b. Let s_0 be the initial state. In our example, we have $n=0$, $w=1$, and b an array of size one in the initial state. We have operations to transform the data structure. In our example, we had operations *pushBack*, *popBack*, and *reallocate*. The application of operation X in a state s transforms the data structure to a new state s' and has cost $T_X(s)$. In our example, the cost of a *pushBack* or *popBack* is 1 excluding the cost of the possible call to *reallocate*. The cost of a call *reallocate*(βn) is $\Theta(n)$.

Let F be a sequence of operations Op_1, Op_2, Op_3, $\ldots$, Op_n. Starting at the initial state s_0, F takes us through a sequence of states to a final state s_n:

$$s_0 \xrightarrow{Op_1} s_1 \xrightarrow{Op_2} s_2 \xrightarrow{Op_3} \cdots \xrightarrow{Op_n} s_n \;.$$

The cost $T(F)$ of F is given by

$$T(F) = \sum_{1 \le i \le n} T_{Op_i}(s_{i-1}) \;.$$

A family of functions $A_X(s)$, one for each operation X, is called a *family of amortized time bounds* if for every sequence F of operations:

$$T(F) \le A(F) := c + \sum_{1 \le i \le n} A_{Op_i}(s_{i-1})$$

for some constant c not depending on F, i.e., up to an additive constant the total actual execution time is bounded by the total amortized execution time.

There is always a trivial way to define a family of amortized time bounds, namely $A_X(s) := T_X(s)$ for all s. The challenge is to find a family of simple functions $A_X(s)$ forming a family of amortized time bounds. In our example, the functions $A_{pushBack}(s) = A_{popBack}(s) = A_{[\cdot]}(s) = \mathcal{O}(1)$ and $A_{reallocate}(s) = 0$ for all s form a family of amortized time bounds.

The Potential or Bank Account Method for Amortized Analysis

We now formalize the technique used in the previous section. We have a function pot that associates a non-negative potential with every state of the data structure, i.e., $pot : S \longrightarrow \mathbb{R}_{\geq 0}$. We call $pot(s)$ the potential of the state s or the balance of the savings account when the data structure is in state s. It requires ingenuity to come up with an appropriate function pot. For an operation X transforming a state s into a state s' and having cost $T_X(s)$, we define the amortized cost $A_X(s)$ as the sum of the potential change and the actual cost, i.e., $A_X(s) = pot(s') - pot(s) + T_X(s)$. The functions obtained in this way form a family of amortized time bounds.

Theorem 8 (Potential Method). *Let S be the set of states of a data structure, let s_0 be the initial state, and let $pot : S \longrightarrow \mathbb{R}_{\geq 0}$ be a non-negative function. For an operation X and a state s with $s \xrightarrow{X} s'$ define*

$$A_X(s) = pot(s') - pot(s) + T_X(s).$$

Then the functions $A_X(s)$ are a family of amortized time bounds.

Proof. A short computation suffices. Consider a sequence $F = \langle Op_1, \ldots, Op_n \rangle$ of operations. We have :

$$\begin{aligned}\sum_{1 \leq i \leq n} A_{Op_i}(s_{i-1}) &= \sum_{1 \leq i \leq n} (pot(s_i) - pot(s_{i-1}) + T_{Op_i}(s_{i-1})) \\ &= pot(s_n) - pot(s_0) + \sum_{1 \leq i \leq n} T_{Op_i}(s_{i-1}) \\ &\geq \sum_{1 \leq i \leq n} T_{Op_i}(s_{i-1}) - pot(s_0),\end{aligned}$$

since $pot(s_n) \geq 0$. Thus $T(F) \leq A(F) + pot(s_0)$.

Let us formulate the analysis of unbounded arrays in the language above. The state of an unbounded array is characterized by the values of n and w. Following Exercise 39, the potential in state (n, w) is $\max(3n - w, w/2)$. The actual costs T of $pushBack$ and $popback$ is one and the actual cost of $reallocate(\beta n)$ is n. The potential of the initial state $(n, w) = (0, 1)$ is $1/2$. A $pushBack$ increases n by one and hence increases the potential by at most three. Thus its amortized cost is bounded by four. A $popBack$ decreases n by one and hence does not increase its potential. Its amortized cost is therefore at most one. The first reallocate occurs when the data structure is in state $(n, w) = (1, 1)$. The potential of this state is $\max(3-1, 1/2) = 2$ and the actual cost of the reallocate is 1. After the reallocate the data structure is in state $(n, w) = (1, 2)$ and has potential $\max(3 - 2, 1) = 1$. Therefore the amortized cost of the first *reallocate* is $1-2+1 = 0$. Consider any other call of *reallocate*. We have either $n = w$ or $4n \leq w$. In the former case, the potential before the reallocate is $2n$, the actual cost is n, the new state is $(n, 2n)$ and has potential n. Thus the amortized cost is $n-2n+n = 0$. In the latter case, the potential before the operation is $w/2$, the actual cost is n which is at most $w/4$ and the new state is $(n, w/2)$ and has potential $w/4$. Thus the amortized cost is at most $w/4 - w/2 + w/4 = 0$. We conclude that the amortized cost of *pushBack* and *popBack* is $\mathcal{O}(1)$ and the amortized cost of *reallocate* is zero or less. Thus a sequence of m operations on an unbounded array has cost $\mathcal{O}(m)$.

Exercise 44 (Amortized analysis of binary counters). Consider a nonnegative integer c represented by an array of binary digits and a sequence of m increment and decrement operations. Initially, $c = 0$. This exercise continues the discussion at the end of Section 3.2.

1. What is the worst case execution time of an increment or a decrement as a function of m? Assume that you can only work at one bit per step.
2. Prove that the amortized cost of increments is constant if there are no decrements. Hint: define the potential of c as the number of ones in the binary representation of c.
3. Give a sequence of m increment and decrement operations with cost $\Theta(m \log m)$.
4. Give a representation of counters such that you can achieve worst case constant time for increment and decrement.
5. Allow each digit d_i to take values from $\{-1, 0, 1\}$. The value of the counter is $c = \sum_i d_i 2^i$. Show that in this *redundant ternary* number system increments and decrements have constant amortized cost. Is there an easy way to tell whether the value of the counter is zero?

Universality of Potential Method

We argue that the potential function technique is strong enough to obtain any family of amortized time bounds.

Theorem 9. *Let $B_X(s)$ be a family of amortized time bounds. Then there is a potential function pot such that $A_X(s) \leq B_X(s)$ for all states s and all operations X where $A_X(s)$ is defined according to the Theorem 8.*

Proof. Let c be such that $T(F) \leq B(F) + c$ for any sequence of operations F starting at the initial state. For any state s we define its potential $pot(s)$ by

$$pot(s) = \inf\{B(F) + c - T(F) : F \text{ is a sequence of operations with final state } s\} .$$

We need to write $\inf$ instead of $\min$, since there might be infinitely many sequences leading to s. We have $pot(s) \geq 0$ for any s since $T(F) \leq B(F) + c$ for any sequence F. Thus pot is a potential function and the functions $A_X(s)$ form a family of amortized time bounds. We need to show $A_X(s) \leq B_X(s)$ for all X and s. Let $\epsilon > 0$ be arbitrary. We show $A_X(s) \leq B_X(s) + \epsilon$. Since ϵ is arbitrary, this proves $A_X(s) \leq B_X(s)$.

Let F be a sequence with final state s and $B(F) + c - T(F) \leq pot(s) + \epsilon$. Let F' be F followed by X, i.e.,

$$s_0 \xrightarrow{F} s \xrightarrow{X} s' \ .$$

Then $pot(s') \leq B(F') + c - T(F')$ by definition of $pot(s')$, $pot(s) \geq B(F) + c - T(F) - \epsilon$ by choice of F, $B(F') = B(F) + B_X(s)$ and $T(F') = T(F) + T_X(s)$ since $F' = F \circ X$, and $A_X(s) = pot(s') - pot(s) + T_X(s)$ by definition of $A_X(s)$. Combining the inequalities we obtain

$$\begin{aligned} A_X(s) &\leq (B(F') + c - T(F')) - (B(F) + c - T(F) - \epsilon) + T_X(s) \\ &= (B(F') - B(F)) - (T(F') - T(F) - T_X(s)) + \epsilon \\ &= B_X(s) + \epsilon \ . \end{aligned}$$

3.4 Stacks and Queues

Sequences are often used in a rather limited way. Let us start with examples from precomputer days. Sometimes a clerk tends to work in the following way: he keeps a *stack* of unprocessed files on his desk. New files are placed on the top of the stack. When he processes the next file he also takes it from the top of the stack. The easy handling of this "data structure" justifies its use; of course, files may stay in the stack for a long time. In the terminology of the preceding sections, a stack is a sequence that only supports the operations $pushBack$, $popBack$, and $last$. We will use the simplified names $push$, pop, and top for the three stack operations.

Behavior is different when people stand in line waiting for service at a post office. Customers join the line at one end and leave it at the other end. Such sequences are called *FIFO queues* (First In First Out) or simply *queues*. In the terminology of the $List$ class, FIFO queues only use the operations $first$, $pushBack$ and $popFront$.

The more general *deque*[1], or *double-ended queue* allows operations $first$, $last$, $pushFront$, $pushBack$, $popFront$ and $popBack$ and can also be observed at a post office, when some not so nice individual jumps the line, or when the clerk at the counter gives priority to a pregnant woman at the end of the line. Figure 3.7 illustrates the access patterns of stacks, queues and deques.

Exercise 45 (The Towers of Hanoi). *In the great temple of Brahma in Benares, on a brass plate under the dome that marks the center of the world, there are 64 disks of pure gold that the priests carry one at a time between these diamond needles according to Brahma's immutable law: no disk may be placed on a smaller disk. In the beginning of the world, all 64 disks formed the Tower of Brahma on one needle.*

[1] Deque is pronounced like "deck".

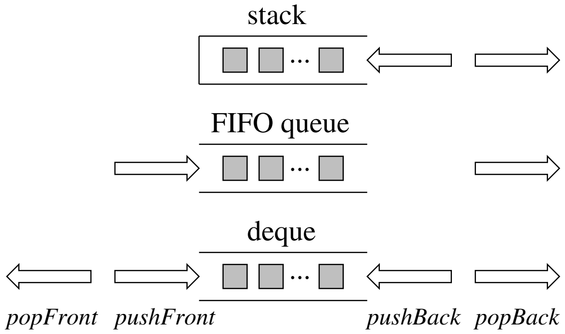


Fig. 3.7. Operations on stacks, queues, and double-ended queues (deques).

Now, however, the process of transfer of the tower from one needle to another is in mid-course. When the last disk is finally in place, once again forming the Tower of Brahma but on a different needle, then the end of the world will come and all will turn to dust. [92].[2]

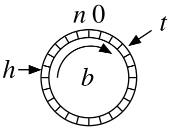
Describe the problem formally for any number k of disks. Write a program that uses three stacks for the poles and produces a sequence of stack operations that transform the state $(\langle k, \ldots, 1\rangle, \langle\rangle, \langle\rangle)$ into the state $(\langle\rangle, \langle\rangle, \langle k, \ldots, 1\rangle)$.

Exercise 46. Explain how to implement a FIFO queue using two stacks so that each FIFO operation takes amortized constant time.

Why should we care about these specialized types of sequences if we already know the list data structure which supports all operations above and more in constant time. There are at least three reasons. First, programs become more readable and are easier to debug if special usage patterns of data structures are made explicit. Second, simple interfaces also allow a wider range of implementations. In particular, the simplicity of stacks and queues allows for specialized implementations that are more space efficient than general $List$s. We will elaborate this algorithmic aspect in the remainder of this section. In particular, we will strive for implementations based on arrays rather than lists. Third, lists are not suited for external memory use because each access to a list item may cause a cache fault. The sequential access patterns to stacks and queues translate into good reuse of cache blocks when stacks and queues are implemented by arrays.

Bounded stacks, where we know the maximal size in advance, are readily implemented with bounded arrays. For unbounded stacks we can use unbounded arrays. Stacks can also be implemented by singly linked lists: the top of the stack corresponds to the front of the list. FIFO queues are easy to realize with singly linked lists with a pointer to the last element. However, deques cannot be implemented efficiently by singly linked lists.

[2] In fact, this mathematical puzzle was invented by the French mathematician Edouard Lucas in 1883.



```
Class BoundedFIFO($n$ : ℕ) of Element
    $b$ : Array $[0..n]$ of Element
    $h = 0$ : ℕ                          // index of first element
    $t = 0$ : ℕ                          // index of first free entry

  Function isEmpty : $\{0,1\}$; return $h = t$

  Function first : Element; assert ¬isEmpty; return $b[h]$

  Function size : ℕ; return $(t - h + n + 1) \bmod (n + 1)$

  Procedure pushBack($x$ : Element)
      assert size$< n$
      $b[t] := x$
      $t := (t + 1) \bmod (n + 1)$

  Procedure popFront assert ¬isEmpty; $h := (h + 1) \bmod (n + 1)$
```

Fig. 3.8. An array-based bounded FIFO queue implementation.

We next discuss an implementation of bounded FIFO queues by arrays, see Figure 3.8. We view the array as a cyclic structure where entry zero follows the last entry. In other words, we have array indices 0 to n and view indices modulo $n + 1$. We maintain two indices h and t delimiting the range of valid queue entries; the queue comprises the array elements indexed h, $h + 1$, ..., $t - 1$. The indices travel around the cycle as elements are queued and dequeued. The cyclic semantics of the indices can be implemented using arithmetics modulo the array size[3]. We always leave at least one entry of the array empty because otherwise it would be difficult to distinguish a full queue from an empty queue. The implementation is readily generalized to bounded deques. Circular arrays also support the random access operator $[\cdot]$.

Operator $[i : \mathbb{N}]$: *Element;* **return** $b[i + h \mathbf{\ mod\ } n]$

Bounded queues and deques can be made unbounded using similar techniques as for unbounded arrays in Section 3.2.

We have now seen the major techniques for implementing stacks, queues and deques. The techniques may be combined to obtain solutions particularly suited for very large sequences or external memory computations.

Exercise 47 (Lists of arrays). Here we want to develop a simple data structure for stacks, FIFO queues, and deques that combines all the advantages of lists and unbounded arrays and is more space efficient for large queues than either of them. Use a list (doubly linked for deques) where each item stores an array of K elements for some large constant K. Implement such a data structure in your favorite programming language. Compare space consumption and execution time to linked lists and unbounded arrays for large stacks.

[3] On some machines one might obtain significant speedups by choosing the array size as a power of two and replacing **mod** by bit operations.

Operation	*List*	*SList*	*UArray*	*CArray*	explanation of '*'
$[\cdot]$	n	n	1	1	
size	1^*	1^*	1	1	not with inter-list *splice*
first	1	1	1	1	
last	1	1	1	1	
insert	1	1^*	n	n	*insertAfter* only
remove	1	1^*	n	n	*removeAfter* only
pushBack	1	1	1^*	1^*	amortized
pushFront	1	1	n	1^*	amortized
popBack	1	n	1^*	1^*	amortized
popFront	1	1	n	1^*	amortized
concat	1	1	n	n	
splice	1	1	n	n	
findNext,...	n	n	n^*	n^*	cache efficient

Table 3.1. Running times of operations on sequences with n elements. Entries have an implicit $\mathcal{O}(\cdot)$ around them. *List* stands for doubly linked lists, *SList* stands for singly linked list, *UArray* stands for unbounded array, and *CArray* stands for circular array.

Exercise 48 (External memory stacks and queues). Design a stack data structure that needs $\mathcal{O}(1/B)$ I/Os per operation in the I/O model from Section 2.2. It suffices to keep two blocks in internal memory. What can happen in a naive implementation with only one block in memory? Adapt your data structure to implement FIFOs, again using two blocks of internal buffer memory. Implement deques using four buffer blocks.

3.5 Lists versus Arrays

Table 3.1 summarizes the findings of this chapter. Arrays are better at indexed access whereas linked lists have their strength in sequence manipulations at arbitrary positions. Both approaches realize the operations needed for stacks and queues efficiently. However, arrays are more cache efficient here whereas lists provide worst case performance guarantees.

Singly linked lists can compete with doubly linked lists in most but not all respects. The only advantage of cyclic arrays over unbounded arrays is that they can implement *pushFront* and *popFront* efficiently.

Space efficiency is also a nontrivial issue. Linked lists are very compact if elements are much larger than pointers. For small *Element* types, arrays are usually more compact because there is no overhead for pointers. This is certainly true if the size of the arrays is known in advance so that bounded arrays can be used. Unbounded arrays have a tradeoff between space efficiency and copying overhead during reallocation.

3.6 Implementation Notes

Every decent programming language supports bounded arrays. Also unbounded arrays, lists, stacks, queues and deques are provided in libraries available for the major imperative languages. Nevertheless, you will often have to implement list-like data structures yourself, e.g., when your objects are members of several linked lists. In such implementations, memory management is often a major challenge.

C++ : The class $vector\langle Element\rangle$ in the STL realizes unbounded arrays. It gives additional control over the allocated size w and is likely to be more efficient than our simple implementation. Usually you will give some initial estimate for the sequence size n when the $vector$ is constructed. This can save you many grow operations. Often, you also know when the array will stop changing size and you can then force $w = n$. With these refinements, there is little reason to use the built-in C style arrays. An added benefit of $vector$s is that they are automatically destructed when the variable gets out of scope. Furthermore, during debugging you may switch to implementations with bound checking.

There are some additional issues that you might want to address if you need very high performance for arrays that grow or shrink a lot. During reallocation, $vector$ has to move array elements using the copy constructor of $Element$. In most cases, a call to the low-level byte copy operation $memcpy$ would be much faster. Another low level optimization is to implement $reallocate$ using the standard C function $realloc$ The memory manager might be able to avoid copying the data entirely.

A stumbling block with unbounded arrays is that pointers to array elements become invalid when the array is reallocated. You should make sure that the array does not change size while such pointers are used. If reallocations cannot be ruled out, you can use array indices rather than pointers.

The STL and LEDA offer doubly linked lists in the class $list\langle Element\rangle$, and singly linked lists in the class $slist\langle Element\rangle$. Their memory management uses free lists for all objects of (roughly) the same size, rather than only for objects of the same class.

If you need to implement a list-like data structure, note that the operator new can be redefined for each class. The standard library class $allocator$ offers an interface that allows you to use your own memory management while cooperating with the memory managers of other classes.

The STL provides classes $stack\langle Element\rangle$ and $deque\langle Element\rangle$ for stacks and double-ended queues, respectively. $Deque$s also allow constant-time indexed access using $[\cdot]$. LEDA offers classes $stack\langle Element\rangle$ and $queue\langle Element\rangle$ for unbounded stacks, and FIFO queues implemented via linked lists. It also offers bounded variants that are implemented as arrays.

Iterators are a central concept of the STL; they implement our abstract view of sequences independent of the particular representation.

Java: The *util* package of the Java 6 platform provides *Vector* for unbounded arrays, *LinkedList* for doubly linked lists. There is a *Deque* interface with implementations by $ArrayDeque$ and $LinkedList$. A $Stack$ is implemented as an extension to $Vector$.

Many Java books proudly announce that Java has no pointers so that you might wonder how to implement linked lists. The solution is that object references in Java are essentially pointers. In a sense, Java has *only* pointers, because members of non-simple type are always references, and are never stored in the parent object itself.

Explicit memory management is optional in Java, since it provides garbage collections of all objects that are not needed any more.

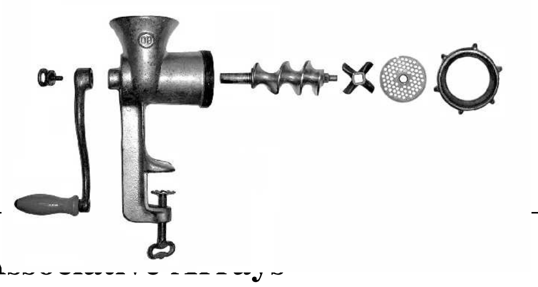
3.7 Historical Notes and Further Findings

All algorithms described in this chapter are *folklore*, i.e., they have been around for a long time and nobody claims to be their inventor. Indeed, we have seen that many of the concepts predate computers.

Amortization is as old as the analysis of algorithms. The *bank account* and the *potential* methods were introduced at the beginning of the 80s by R.E. Brown, S. Huddlestone, K. Mehlhorn, D.D. Sleator, and R.E. Tarjan [32, 93, 170, 171]. The overview article [176] popularized the term *amortized analysis* and Theorem 9 first appeared in [123].

There is an array-like data structure that supports indexed access in constant time and arbitrary element insertion and deletion in amortized time $\mathcal{O}(\sqrt{n})$. The trick is relatively simple. The array is split into subarrays of size $n' = \Theta(\sqrt{n})$. Only the last subarray may contain less elements. The subarrays are maintained as cyclic arrays as described in Section 3.4. Element i can be found in entry $i \mathbf{\ mod\ } n'$ of subarray $\lfloor i/n' \rfloor$. A new element is inserted in its subarray in time $\mathcal{O}(\sqrt{n})$. To repair the invariant that subarrays have the same size, the last element of this subarray is inserted as the first element of the next subarray in constant time. This process of shifting the extra element is repeated $\mathcal{O}(n/n') = \mathcal{O}(\sqrt{n})$ times until the last subarray is reached. Deletion works similarly. Occasionally, one has to start a new last subarray or change n' and reallocate everything. The amortized cost of these additional operations can be kept small. With some additional modifications, all deque operations can be performed in constant time. We refer the reader to [104] for more sophisticated implementations of deques and an implementation study.

4



Hash Tables and Associative Arrays

[ps:Das Bild ist aus Wikipedia. Ich habe auch eine hÃűherauflÃűsende Variante] *If you want to get a book from the central library of the University of* ⟸ *Karlsruhe, you have to order the book an hour in advance. The library personnel fetches the book from the stack and delivers it to a room with 100 shelves. You find your book in a shelf numbered with the* last *two digits of your library card. Why the last digits and not the leading digits? Probably, because this distributes the books more evenly about the shelves. The library cards are numbered consecutively as students sign up and the University of Karlsruhe was founded in 1825. Therefore, the students enrolled at the same time are likely to have the same leading digits in their card number and only a few shelves would be in use.*

The subject of this chapter is the robust and efficient implementation of the above "delivery shelf data structure". In Computer Science the data structure is known as a *hash table*. Hash tables are one implementation of *associative arrays* or *dictionaries*. The other implementation are tree data structures which we will study in Chapter 7. An associative array is an array with a potentially infinite or at least very large index set out of which only a small number of indices are actually in use. For example, the potential indices are all strings and the indices in use are all identifiers used in a particular C++ program. Or the potential indices are all ways of placing chess pieces on a chess board and the indices in use are the placements required in the analysis of a particular game. Associative arrays are versatile data structures. Compilers use them for their *symbol table* that associates identifiers with information about them. Combinatorial search programs often use them for detecting whether a situation was already looked at. For example, chess programs have to deal with the fact that board positions can be reached by different sequences of moves. However, each position should be evaluated only once. The solution is to store positions in an associate array. One of the most widely used implementations of the *join*-operation in relational databases temporarily stores one of the participating relations in an associative array. Scripting languages such as `awk` [6] or `perl` [190] use associative arrays as their *only* data structure. In all examples above, the associate array is usually implemented as a hash table. The exercises of this section ask you to work out some uses of associative arrays.

Formally, an associative array S stores a set of elements. Each element e has an associated key $key(e) \in Key$. We assume keys to be unique, i.e., distinct elements have distinct keys. Associative arrays support the following operations:

$S.insert(e : Element)$: $S := S \cup \{e\}$
$S.remove(k : Key)$: $S := S \setminus \{e\}$ where e is the unique element with $key(k) = k$.
$S.find(k : Key)$: If there is an $e \in S$ with $key(k) = k$ return e otherwise return $\perp$.

In addition, we assume a mechanism that allows us to retrieve all elements in S. Since this *forall* operation is usually easy to implement, we only discuss it in the exercises. Observe that the *find*-operation is essentially the random access operator in an array; therefore, the name associative array. Key is the set of potential array indices and the elements in S are the indices in use at any particular time. Throughout this chapter, we use n to denote the size of S and N to denote the size of Key. In a typical application of associative arrays, N is humongous and hence the usage of an array of size N is out of the question. We are aiming for solutions which use space $O(n)$.

In the library example, Key is the set of all library card numbers and elements are the book orders. Another pre-computer example is an English-German dictionary. The keys are English words and an element is an English word together with its German translations.

The basic idea behind the hash table implementation of associative arrays is simple. We use a so-called *hash function* h to map the set Key of potential array indices to a small range $[0..m-1]$ of integers. We also have an array t with index set $[0..m-1]$, the so-called *hash table*. In order to keep the space requirement low, we want m to be about the number of elements in S. The hash function associates with each element e a *hash value* $h(key(e))$. In order to simplify notation, we write $h(e)$ instead of $h(key(e))$ for the hash value of e. In the library example, h maps each library card number to its last two digits. Ideally, we would like to store element e in table entry $t[h(e)]$. If this works, we obtain constant execution time[1] for our three operations $insert$, $remove$, and $find$.

Unfortunately, storing e in $t[h(e)]$ will not always work as several elements might *collide*, i.e., map to the same table entry. The library examples suggests a fix: Allow several book orders to go to the same shelf. Then the entire shelf has to be searched to find a particular order. The generalization of this fix leads to *hashing with chaining*. We store a set of elements in each table entry and implement the set using singly linked lists. Section 4.1 analyzes hashing with chaining using rather optimistic (and hence unrealistic) assumptions about the properties of the hash function. In this model, we achieve constant expected time for all three dictionary operations.

In Section 4.2 we drop the unrealistic assumptions and construct hash functions that come with (probabilistic) performance guarantees. Already our simple examples show that finding good hash functions is non-trivial. For example, if we apply the

[1] Strictly speaking, we have to add additional terms for evaluating the hash function and for moving elements around. To simplify notation, we assume in this chapter that all of this takes constant time.

least significant digit idea from the library example to an English-German dictionary, we might come up with a hash function based on the last four letters of a word. But then we would have lots of collisions for words ending on ‘tion’, ‘able’, etc.

We can simplify hash tables (but not their analysis) by returning to the original idea of storing all elements in the table itself. When a newly inserted element e finds entry $t[h(x)]$ occupied, it scans the table until a free entry is found. In the library example, assume that shelves can hold exactly one book. The librarians would then use the adjacent shelves to store books that map to the same delivery shelf. Section 4.3 elaborates on this idea, which is known as *hashing with open addressing and linear probing*.

Why are hash tables called hash tables? The dictionary explains “to hash” as “to chop up, as of potatoes”. This is exactly, what hash functions usually do. For example, if keys are strings, the hash function may chop up the string into pieces of fixed size, interpret each fixed-size piece as a number, and then compute a single number from the sequence of numbers. A good hash function creates disorder and in this way avoids collisions.

Exercise 49. Assume you are given a set M of pairs of integers. M defines a binary relation R_M. Use an associative array to check whether R_M is symmetric. A relation is symmetric if $\forall(a,b) \in M : (b,a) \in M$.

Exercise 50. Write a program that reads a text file and outputs the 100 most frequent words in the text.

Exercise 51 (A billing system:). Assume you have a large file consisting of triples (transaction, price, customer ID). Explain how to compute the total payment due for each customer. Your algorithm should run in linear time.

Exercise 52 (Scanning a hash table.). Show how to realize the *forall* operation for hashing with chaining and hashing with open addressing and linear probing. What is the running time of your solution?

4.1 Hashing with Chaining

Hashing with chaining maintains an array t of linear lists, see Figure 4.1. The associative array operations are easy to implement. To insert an element e, we insert it somewhere in sequence $t[h(e)]$. To remove the element with key k, we scan through $t[h(k)]$. If an element e with $h(e) = k$ is encountered, we remove it and return. To find the element with key k, we also scan through $t[h(k)]$. If an element e with $h(e) = k$ is encountered, we return it. Otherwise, we return $\perp$.

Insertions take constant time. Space consumption is $\mathcal{O}(n + m)$. To remove or find a key k, we have to scan the sequence $t[h(k)]$. In the worst case, for example, if *find* looks for an element that is not there, the entire list has to be scanned. If we are unlucky, all elements are mapped to the same table entry and the execution time is $\Theta(n)$. So in the worst case hashing with chaining is no better than linear lists.

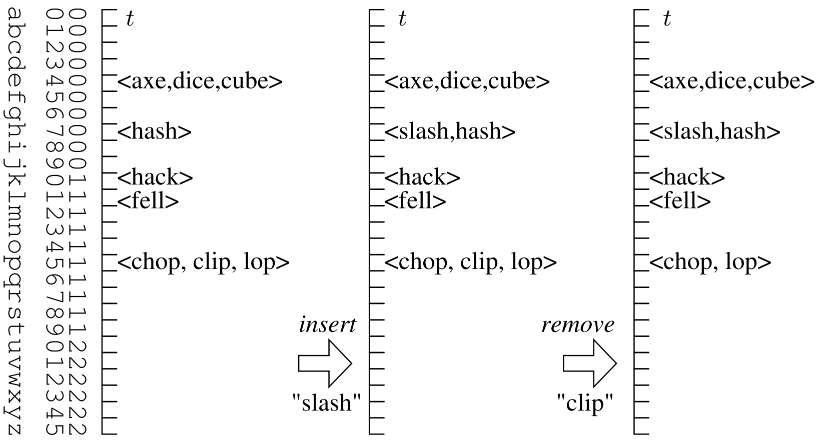


Fig. 4.1. Hashing with chaining. We have a table t of sequences. The picture shows an example where a set of words (short synonyms of 'hash') is stored using a hash function that maps the last character to the integers $0..25$. We see that this hash function is not very good.

Are there hash functions that guarantee that all sequences are short? The answer is clearly no. A hash function maps the set of keys to the range $[0..m-1]$ and hence for every hash function there is always a set of N/m keys that all map to the same table entry. In most applications, $n < N/m$ and hence hashing can always deteriorate to linear search. We will study three approaches to dealing with the worst case behavior. The first approach is average case analysis. In Exercise 55 we will ask you to argue that random sets of keys fare well. The second approach is to use randomization and to choose the hash function at random from a collection of hash functions. We will study this approach in this section and the next. The third approach is to change the algorithm. For example, we could make the hash function depend on the set of keys in actual use. We will investigate this approach in Section 4.5 and show that it leads to good worst case behavior.

Let H be the set of all functions from Key to $[0..m-1]$. We assume that the hash function h is chosen randomly[2] from H and show that for any fixed set S of n keys, the expected execution time of $remove$ or $find$ will be $\mathcal{O}(1 + n/m)$.

Theorem 10. *If n elements are stored in a hash table with m entries and a random hash function is used, the expected execution time of remove or find is $\mathcal{O}(1 + n/m)$.*

Proof. The proof requires the probabilistic concepts of random variables, their expectation, and linearity of expectation as described in Appendix A.2. Consider the execution time of $remove$ or $find$ for a fixed key k. Both need constant time plus

[2] This assumption is completely unrealistic. There are m^N functions in H and hence it requires $N \log m$ bits to specify a function in H. This defeats the goal of reducing the space requirement from N to n.

the time for scanning the sequence $t[h(k)]$. Hence the expected execution time is $\mathcal{O}(1 + \mathrm{E}[X])$ where the random variable X stands for the length of sequence $t[h(k)]$. Let S be the set of n elements stored in the hash table. For each $e \in S$, let X_e be the *indicator* variable which tells us whether e hashes to the same location as k, i.e., $X_e = 1$ if $h(e) = h(k)$ and $X_e = 0$ otherwise. In short hand, $X_e = [h(e) = h(k)]$. We have $X = \sum_{e \in S} X_e$. Using linearity of expectation, we obtain

$$\mathrm{E}[X] = \mathrm{E}[\sum_{e\in S} X_e] = \sum_{e\in S} \mathrm{E}[X_e] = \sum_{e\in S} \mathrm{prob}(X_i = 1) \ .$$

A random hash function maps e to all m table entries with the same probability, independent of $h(k)$. Hence, $\mathrm{prob}(X_e = 1) = 1/m$ and therefore $\mathrm{E}[X] = n/m$. Thus, the expected execution time of *find* and $remove$ is $\mathcal{O}(1 + n/m)$.

We can achieve linear space requirement and constant expected execution time of all three operations by guaranteeing $m = \Theta(n)$ at all times. Adaptive reallocation as described for unbounded arrays in Section 3.2 is the appropriate technique.

Exercise 53 (Unbounded Hash Tables). Explain how to guranatee $m = \Theta(n)$ in hashing with chaining. You may assume the existence of a hash function $h' : Key \to \mathbb{N}$. Set $h(k) = h'(k) \bmod m$ and use adaptive reallocation.

Exercise 54 (Waste of space). Waste of space in hashing with chaining is due to empty table entries. Assuming a random hash function, compute the expected number of empty table entries as a function of m and n. Hint: Define indicator random variables $Y_0, \ldots, Y_{m-1}$ where $Y_i = 1$ if $t[i]$ is empty.

Exercise 55 (Average Case Behavior). Assume that the hash function distributes Key evenly over the table, i.e., for each i, $0 \le i \le m{-}1$, we have $|\,\{k \in Key : h(k) = i\}\,| \le \lceil N/m \rceil$. Assume that a random set S of n keys is stored in the table, i.e., S is a random subset of Key of size n. Show that for any table position i, the expected number of elements in S hashing to i is at most $\lceil N/m \rceil \cdot n/N \approx n/m$.

4.2 Universal Hash Functions

Theorem 10 is unsatisfactory as it presupposes that the hash function is chosen randomly from the set of all functions[3] from keys to table positions. The class of all such functions is much too big to be useful. We will show in this section that the same performance can be obtained with much smaller classes of hash functions. The families presented in this section are so small that a member can be specified in constant space. Moreover, the functions are easy to evaluate.

[3] We will usually talk about a class of functions or a family of functions in this chapter and reserve the word set for the set of keys stored in the hash table.

Definition 1. *Let c be a positive constant. A family H of functions from Key to $[0..m-1]$ is called* c-universal *if any two distinct keys collide with probability at most c/m, i.e., for all x, y in Key with $x \neq y$*

$$|\{h \in H : h(x) = h(y)\}| \leq \frac{c}{m}|H| \, .$$

In other words, for random $h \in H$,

$$\mathrm{prob}(h(x) = h(y)) \leq \frac{c}{m} \, .$$

The definition is made such that the proof of Theorem 10 extends.

Theorem 11. *If n elements are stored in a hash table with m entries using hashing with chaining and a random hash function from a c-universal family is used, the expected execution time of $remove$ or find is $\mathcal{O}(1 + cn/m)$.*

Proof. We can reuse the proof of Theorem 10 almost literally. Consider the execution time of $remove$ or *find* for a fixed key k. Both need constant time plus the time for scanning the sequence $t[h(k)]$. Hence the expected execution time is $\mathcal{O}(1 + \mathrm{E}[X])$ where the random variable X stands for the length of sequence $t[h(k)]$. Let S be the set of n elements stored in the hash table. For each $e \in S$, let X_e be the *indicator* variable which tells us whether e hashes to the same location as k, i.e., $X_e = 1$ if $h(e) = h(k)$ and $X_e = 0$ otherwise. In short hand, $X_e = (h(e) = h(k))$. We have $X = \sum_{e \in S} X_e$. Using linearity of expectation, we obtain

$$\mathrm{E}[X] = \mathrm{E}[\sum_{e \in S} X_e] = \sum_{e \in S} \mathrm{E}[X_e] = \sum_{e \in S} \mathrm{prob}(X_i = 1) \ \ .$$

Since h is chosen uniformly from a c-universal class, we have $\mathrm{prob}(X_e = 1) \leq c/m$ and hence $\mathrm{E}[X] = cn/m$. Thus, the expected execution time of *find* and $remove$ is $\mathcal{O}(1 + cn/m)$.

Now it remains to find c-universal families of hash functions that are easy to construct and easy to evaluate. We explain a simple and quite practical 1-universal family in detail and give further examples in the exercises. We assume that our keys are bitstrings of a certain fixed length; in the exercises, we discuss how the fixed length assumption can be overcome. We also assume that the table size m is a prime number. Why a prime number? Because arithmetic modulo a prime is particularly nice, in particular, the set $\mathbb{Z}_m = \{0, \ldots, m-1\}$ of numbers modulo m form a field[4]. Let $w = \lfloor \log m \rfloor$. We subdivide the keys into pieces of w bits each, say k pieces. We interpret each piece as an integer in the range $[0..2^w - 1]$ and keys as k-tuples of such integers. For a key $\mathbf{x}$ we write $\mathbf{x} = (x_1, \ldots, x_k)$ to denote its partition into pieces. Each x_i lies in $[0..2^w - 1]$. We can now define our class of hash functions. For each

[4] A field is a set with special elements 0 and 1 and operations addition and multiplication. Addition and multiplication satisfy the usual laws known from the field of rational numbers.

$\mathbf{a} = (a_1, \ldots, a_k) \in \{0..m-1\}^k$ we define a function $h_{\mathbf{a}}$ from Key to $\{0..m-1\}$ as follows. Let $\mathbf{x} = (x_1, \ldots, x_k)$ be a key and let $\mathbf{a} \cdot \mathbf{x} = \sum_{i=1}^{k} a_i x_i$ denote the scalar product of $\mathbf{a}$ and $\mathbf{x}$. Then

$$h_{\mathbf{a}}(x) = \mathbf{a} \cdot \mathbf{x} \bmod m \; .$$

We give an example to clarify the definition. Let $m = 17$ and $k = 4$. Then $w = 4$ and we view keys as 4-tuples of integers in the range $[0..15]$, for example $\mathbf{x} = (11, 7, 4, 3)$. A hash function is specified by a 4-tuple of integers in the range $[0..16]$, e.g., $\mathbf{a} = (2, 4, 7, 16)$. Then $h_{\mathbf{a}}(\mathbf{x}) = (2 \cdot 11 + 4 \cdot 7 + 7 \cdot 4 + 16 \cdot 3) \bmod 17 = 7$.

Theorem 12.

$$H^{\cdot} = \left\{ h_{\mathbf{a}} : \mathbf{a} \in \{0..m-1\}^k \right\}$$

is a 1-universal family of hash functions if m is prime.

In other words, the scalar product between a tuple representation of a key and a random vector defines a good hash function.

Proof. Consider two distinct keys $\mathbf{x} = (x_1, \ldots, x_k)$ and $\mathbf{y} = (y_1, \ldots, y_k)$. To determine $\mathrm{prob}(h_{\mathbf{a}}(x) = h_{\mathbf{a}}(\mathbf{y}))$, we count the number of choices for $\mathbf{a}$ such that $h_{\mathbf{a}}(\mathbf{x}) = h_{\mathbf{a}}(\mathbf{y})$. Fix an index j such that $x_j \neq y_j$. Then $(x_j - y_j) \not\equiv 0 (\mathrm{mod} m)$ and hence any equation of the form $a_j(x_j - y_j) = b (\mathrm{mod} m)$ where $b \in \mathbb{Z}_m$ has a unique solution in a_j, namely $a_j = (x_j - y_j)^{-1} b (\mathrm{mod} m)$. Here $(x_j - y_j)^{-1}$ denotes the *multiplicative inverse*[5] of $(x_j - y_j)$.

We claim that for each choice of the a_i's with $i \neq j$ there is exacly one choice of a_j such that $h_{\mathbf{a}}(\mathbf{x}) = h_{\mathbf{a}}(\mathbf{y})$. We have

$$\begin{aligned} h_{\mathbf{a}}(\mathbf{x}) = h_{\mathbf{a}}(\mathbf{y}) \Leftrightarrow & \sum_{1 \leq i \leq k} a_i x_i \equiv \sum_{1 \leq i \leq k} a_i y_i & (\mathrm{mod} m) \\ \Leftrightarrow & \; a_j(x_j - y_j) \equiv \sum_{i \neq j} a_i(y_i - x_i) & (\mathrm{mod} m) \\ \Leftrightarrow & \qquad a_j \equiv (y_j - x_j)^{-1} \sum_{i \neq j} a_i(x_i - y_i) & (\mathrm{mod} m). \end{aligned}$$

There are m^{k-1} ways to choose the a_i with $i \neq j$ and for each such choice there is a unique choice for a_j. Since the total number of choices for $\mathbf{a}$ is m^k, we obtain

$$\mathrm{prob}(h_{\mathbf{a}}(x) = h_{\mathbf{a}}(\mathbf{y})) = \frac{m^{k-1}}{m^k} = \frac{1}{m} \; .$$

Is it a serious restriction that we need prime table sizes? At a first glance, yes. We certainly cannot burden users with the task of providing appropriate primes. Also, when we adaptively grow or shrink an array, it is not clear how to get prime numbers for the new value of m. A closer look shows that the problem is easy to resolve.

[5] In a field, any element $z \neq 0$ has a unique multiplicative inverse, i.e., there is a unique element z^{-1} such that $z^{-1} \cdot = 1$. Multiplicative inverses allow to solve linear equations of the form $zx = b$ where $z \neq 0$. The solution is $x = z^{-1} b$.

The easiest solution is to consult a table of primes. An analytical solution is not much harder to obtain. First, number theory [81] tells us that primes are abundant. More precisely, for any integer k there is a prime in the interval $[k^3, (k+1)^3]$. So, if we are aiming for a table size of about m, we determine k such that $k^3 \leq m \leq (k+1)^3$ and then search for a prime in the interval. How do we search for a prime in the interval? Any non-prime in the interval must have a divisor which is at most $\sqrt{(k+1)^3} = (k+1)^{3/2}$. We therefore iterate over the numbers from 1 to $(k+1)^{3/2}$ and for each such j remove its multiples in $[k^3, (k+1)^3]$. For each fixed j this takes time $((k+1)^3 - k^3)/j = \mathcal{O}\big(k^2/j\big)$. The total time required is

$$\begin{aligned}\sum_{j \leq (k+1)^{3/2}} \mathcal{O}\left(\frac{k^2}{j}\right) &= k^2 \sum_{j \leq (k+1)^{3/2}} \mathcal{O}\left(\frac{1}{k}\right) \\ &= \mathcal{O}\Big(k^2 \ln\big((k+1)^{3/2}\big)\Big) = \mathcal{O}\big(k^2 \ln k\big) = o(m)\end{aligned}$$

and hence is negligable compared to the cost of initializing a table of size m. The second equality in the equation above uses the *harmonic* summation formula (A.12).

Exercise 56 (Strings as keys.). Implement the universal family $H^{\cdot}$ for strings. Assume that each character requires eight bits (= a byte). You may assume that the table size is at least $m = 257$. The time for evaluating a hash function should be proportional to the length of the string being processed. Input strings may have arbitrary lengths not known in advance. Hint: compute the random vector $\mathbf{a}$ lazily, extending it only when needed.

$\Longrightarrow$ **Exercise 57 (Hashing using bit matrix multiplication.).** [Literatur? Martin fragen] For this exercise, keys are bit strings of length k, i.e., $Key = \{0,1\}^k$, and the table size m is a power of two, say $m = 2^w$. Each $w \times k$ matrix M with entries in $\{0,1\}$ defines a hash function h_M. For $x \in \{0,1\}^k$, let $h_M(x) = Mx \bmod 2$, i.e., $h_M(x)$ is matrix-vector product computed modulo 2. The resulting w-bit vector is interpreted as a number in $[0 \ldots m-1]$. Let

$$H^{\oplus} = \left\{ h_M : M \in \{0,1\}^{w \times k} \right\} .$$

For $M = \left(\begin{smallmatrix}1&0&1&1\\0&1&1&1\end{smallmatrix}\right)$ and $x = (1,0,0,1)$ we have $Mx \bmod 2 = (0,1)$. Note that multiplication modulo two is the logical and-operation, and that addition modulo two is the logical exclusive-or operation $\oplus$.

1. Explain how $h_M(x)$ can be evaluated using k bit-parallel exclusive-or operations. Hint: the ones in x select columns of M. Add the selected columns.
2. Explain how $h_M(x)$ can be evaluated using w bit-parallel and operations and w $parity$ operations. Many machines provide an instruction $parity(y)$ that is one if the number of ones in y is odd and zero otherwise. Hint: multiply each row of M with x.

3. We now want to show that $H^{\oplus}$ is 1-universal. (1) Show that for any two keys $x \neq y$, any bit position j where x and y differ, and any choice of the columns M_i of the matrix with $i \neq j$, there is exactly one choice of column M_j such that $h_M(x) = h_M(y)$. (2) Count the number of ways to choose $k-1$ columns of M. (3) Count the total number of ways to choose M. (4) Compute the probability $\mathrm{prob}(h_M(x) = h_M(y))$ for $x \neq y$ if M is chosen randomly.

***Exercise 58 (More matrix multiplication.)** Define a class of hash functions

$$H^{\times} = \left\{ h_M : M \in \{0..p\}^{w \times k} \right\}$$

that generalizes class $H^{\oplus}$ by using arithmetic modulo p for some prime number p. Show that $H^{\times}$ is 1-universal. Explain how $H^{\cdot}$ is a special case of $H^{\times}$.

Exercise 59 (Simple linear hash functions.). Assume $Key = [0..p-1] = \mathbb{Z}_p$ for some prime number p. For $a, b \in \mathbb{Z}_p$ let $h_{(a,b)}(x) = ((ax+b) \bmod p) \bmod m$. For example, if $p = 97$, $m = 8$, we have $h_{(23,73)}(2) = ((23 \cdot 2 + 73) \bmod 97) \bmod 8 = 22 \bmod 8 = 6$. Let

$$H^{*} = \left\{ h_{(a,b)} : a, b \in [0..p-1] \right\} .$$

Show that this family is $(\lceil p/m \rceil / (p/m))^2$-universal.

Exercise 60 (Continuation.). Show that the following holds for the class H^{*} defined in the previous exercise. For any pair of distinct keys x and y and any i and j in $[0..m-1]$, $\mathrm{prob}(h_{(a,b)}(x) = i$ and $h_{(a,b)}(y) = j) \leq c/m^2$ for some constant c.

Exercise 61 (A counterexample.). Let $Key = [0..p-1]$ and consider the set of hash functions

$$H^{\mathrm{fool}} = \left\{ h_{(a,b)} : a, b \in [0..p-1] \right\}$$

with $h_{(a,b)}(x) = (ax+b) \bmod m$. Show that there is a set S of $\lceil p/m \rceil$ keys such that for any two keys x and y in S, all functions in H^{fool} map x and y to the same value. Hint: Let $S = \{0, m, 2m, \ldots, \lfloor p/m \rfloor m\}$.

Exercise 62 (Table size 2^{ℓ}.). Let $Key = [0..2^k - 1]$. Show that the family of hash functions

$$H^{\gg} = \left\{ h_a : 0 < a < 2^k \wedge a \text{ is odd} \right\}$$

with $h_a(x) = (ax \bmod 2^k) \operatorname{div} 2^{k-\ell}$ is 2-universal.

Exercise 63 (Table lookup.). Let $m = 2^w$ and view keys as $k+1$-tuples where the 0-th element is a w-bit number and the remaining elements are a-bit numbers for some small constant a. A hash function is defined by tables t_1 to t_k, each having size $s = 2^a$ and storing bit-strings of length w. Then

$$h_{\oplus(t_1,\ldots,t_k)}((x_0, x_1, \ldots, x_k)) = x_0 \oplus \bigoplus_{i=1}^{k} t_i[x_i] ,$$

i.e., x_i selects an element in table t_i and then the bitwise exlusive-or of x_0 and the $t_i[x_i]$ is formed. Show that

$$H^{\oplus[]} = \left\{h_{(t_1,\dots,t_k)} : t_i \in \{0..m-1\}^s\right\}$$

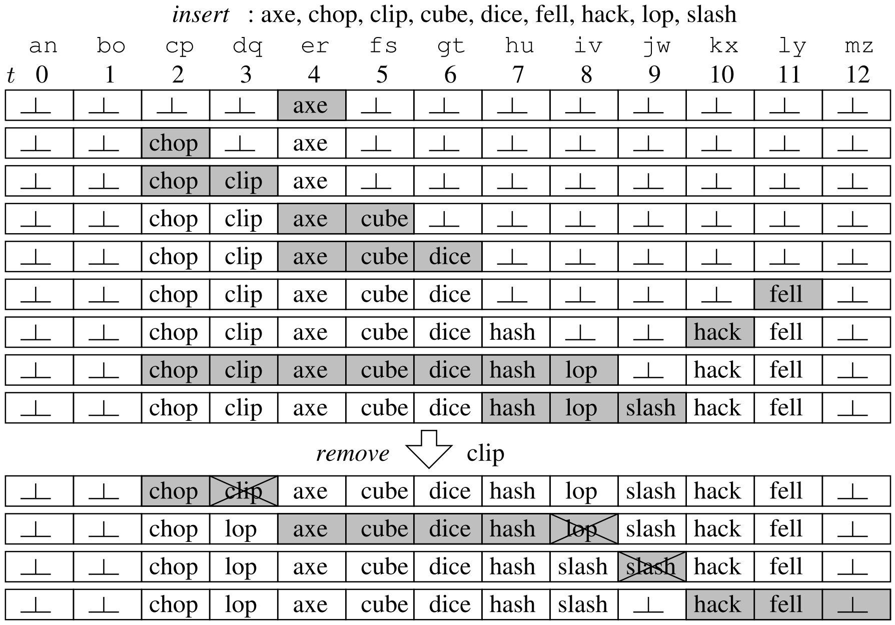
is 1-universal.

4.3 Hashing with Linear Probing

Hashing with chaining is categorized as a *closed* hashing approach because each table entry has to cope with all elements hashing to it. In contrast, *open* hashing schemes open up other table entries to take the overflow from overloaded fellow entries. This added flexibility allows us to do away with secondary data structures such as linked lists—all elements are stored directly in table entries. Many ways of organizing open hashing have been investigated. We will only explore the simplest scheme. Unused entries are filled with a special element $\perp$. An element e is stored in entry $t[h(e)]$ or further to the right. But we only go away from index $h(e)$ with good reason: if e is stored in $t[i]$ with $i > h(e)$ then positions $h(e)$ to $i-1$ are occupied by other elements.

The implementation of insert and find is trivial. To insert an element e, we linearly scan the table starting at $t[h(e)]$ until a free entry is found, where e is then stored. Figure 4.2 gives an example. Similarly, to find an element e, we scan the table starting at $t[h(e)]$ until the element is found. The search is aborted when an empty table entry is encountered. So far this sounds easy enough, but we have to deal with one complication. What happens if we reach the end of the table during insertion? We choose a very simple fix by allocating m' table entries to the right of the largest index produced by the hash function h. For 'benign' hash functions it should be sufficient to choose m' much smaller than m in order to avoid table overflows. Alternatively, one may treat the table as a cyclic array, see Exercise 64 and Section 3.4. The alternative is more robust but slightly slower.

The implementation of $remove$ is non-trivial. Simply overwriting the element by $\perp$ does not suffice as it may destroy the invariant. Assume $h(x) = h(z)$, $h(y) = h(x)+1$ and x, y and z are inserted in this order. Then z is stored at position $h(x)+2$. Overwriting y by $\perp$ will make z inaccessible. There are three solutions. First, disallow removals. Second, mark y but do not actually remove it. Searches are only allowed to stop at $\perp$, but not at marked elements. The problem with this approach is that the number of nonempty cells (occupied or marked) keeps increasing, so searches eventually become slow. This can only be mitigated by introducing the additional complication of periodic reorganizations of the table. Third, actively restore the invariant. Assume that we want to remove the element at i. We overwrite it by $\perp$ leaving a "hole". We then scan the entries to the right of i to check for violations of the invariant. Set j to $i+1$. If $t[j] = \perp$, we are finished. Otherwise, let f be the element stored in $t[j]$. If $h(f) > i$, there is nothing to do and we increment j. If $h(f) \leq i$, leaving the hole would violate the invariant and f would not be found



insert : axe, chop, clip, cube, dice, fell, hack, lop, slash

	an	bo	cp	dq	er	fs	gt	hu	iv	jw	kx	ly	mz
t	0	1	2	3	4	5	6	7	8	9	10	11	12
	⊥	⊥	⊥	⊥	axe	⊥	⊥	⊥	⊥	⊥	⊥	⊥	⊥
	⊥	⊥	chop	⊥	axe	⊥	⊥	⊥	⊥	⊥	⊥	⊥	⊥
	⊥	⊥	chop	clip	axe	⊥	⊥	⊥	⊥	⊥	⊥	⊥	⊥
	⊥	⊥	chop	clip	axe	cube	⊥	⊥	⊥	⊥	⊥	⊥	⊥
	⊥	⊥	chop	clip	axe	cube	dice	⊥	⊥	⊥	⊥	⊥	⊥
	⊥	⊥	chop	clip	axe	cube	dice	⊥	⊥	⊥	⊥	fell	⊥
	⊥	⊥	chop	clip	axe	cube	dice	hash	⊥	⊥	hack	fell	⊥
	⊥	⊥	chop	clip	axe	cube	dice	hash	lop	⊥	hack	fell	⊥
	⊥	⊥	chop	clip	axe	cube	dice	hash	lop	slash	hack	fell	⊥

remove ⇩ clip

⊥	⊥	chop	~~clip~~	axe	cube	dice	hash	lop	slash	hack	fell	⊥
⊥	⊥	chop	lop	axe	cube	dice	hash	~~lop~~	slash	hack	fell	⊥
⊥	⊥	chop	lop	axe	cube	dice	hash	slash	~~slash~~	hack	fell	⊥
⊥	⊥	chop	lop	axe	cube	dice	hash	slash	⊥	hack	fell	⊥

Fig. 4.2. Hashing with linear probing. We have a table t with 13 entries storing synonyms of 'hash'. The hash function maps the last character of the word to the integers $0..12$ as indicated above the table: a and n are mapped to 0, b and o are mapped to 1, and so on. First, the words are inserted in alphabetical order. Then 'clip' is removed. The picture shows the state changes of the table. Gray areas show the range that is scanned between the state changes.

anymore. We therefore move f to $t[i]$ and write $\perp$ into $t[j]$. In other words, we swap f and the hole. We set the hole position i to its new position j and continue with $j := j + 1$. Figure 4.2 gives an example.

Exercise 64 (Cyclic linear probing.). Implement a variant of linear probing where the table size is m rather than $m+m'$. To avoid overflow at the right end of the array, make probing wrap around. (1) Adapt insert and remove by replacing increments with $i := i + 1 \bmod m$. (2) Specify a predicate $\mathit{between}(i, j, k)$ that is true if and only if j is cyclically between i and j. (3) Reformulate the invariant using $\mathit{between}$. (4) Adapt remove.

Exercise 65 (Unbounded linear probing.). Implement unbounded hash tables using linear probing and universal hash functions. Pick a new random hash function whenever the table is reallocated. Let $1 < \gamma < \beta < \alpha$ denote constants we are free to choose. Keep track of the number of stored elements n. Expand the table to $m = \beta n$ if $n > m/\gamma$. Shrink the table to $m = \beta n$ if $n < m/\alpha$. If you do not use cyclic probing as in Exercise 64, set $m' = \delta m$ for some $\delta < 1$ and reallocate the table if the right end should overflow.

4.4 Chaining Versus Linear Probing

We have seen two different approaches to hash tables, chaining and linear probing. Which one is better? This question is beyond theoretical analysis as the answer depends on the intended use and many technical parameters. We therefore discuss some qualitative issues and report about experiments performed by us.

An advantage of chaining is referential integrity. Subsequent find operations for the same element will return the same location in memory and hence references to the results of find operations can be established. In constrast, removal of an element in linear probing may move other elements and hence invalidate references to them.

An advantage of linear probing is that, in each table access, a contiguous piece of memory is accessed. The memory subsystems of modern processors are optimized for this kind of access pattern, whereas they are quite slow at chasing pointers when the data does not fit in cache memory. A disadvantage of linear probing is that search times become high when the number of elements approaches the table size. For chaining, the expected access time remains small. On the other hand, chaining wastes space for pointers that could be used to support a larger table in linear probing. A fair comparison must be based on space consumption and not just on table size.

We implemented both approaches and performed extensive experiments. The outcome is that both techniques perform almost equally well when they are given the same amount of memory. The differences are so small that details of the implementation, compiler, operating system and machine used can reverse the picture. Hence we do not report exact figures.

However, we found chaining harder to implement. Only the optimizations discussed in Section 4.6 make it competitive with linear probing. Chaining is much slower if the implementation is sloppy or memory management is not implemented well.

4.*5 Perfect Hashing

The hashing schemes discussed so far guarantee only *expected* constant time for operations find, insert, and remove. This makes them unsuitable for real-time applications requiring a worst case guarantee. In this section, we will study *perfect hashing* which guarantees constant worst case for find. To keep things simple, we will restrict ourselves to the *static* case where we consider a fixed set S of n elements with keys k_1 to k_n.

In this section, we use H_m to denote a family of c-universal hash functions with range $[0..m-1]$. In Exercise 59 it is shown that 2-universal classes exist for every m. For $h \in H_m$ we use $C(h)$ to denote the number of collisions produced by h, i.e., the number of pairs of distinct keys in S which are mapped to the same position:

$$C(h) = \{(x,y) : x, y \in S,\ x \neq y \text{ and } h(x) = h(y)\} \ .$$

As a first step we derive a bound on the expectation of $C(h)$.

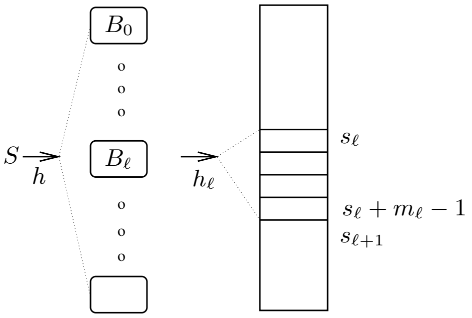


Fig. 4.3. Perfect hashing. The top level hash function h splits S into subsets $B_0, \ldots, B_\ell, \ldots$. Let $b_\ell = |B_\ell|$ and $m_\ell = cb_\ell(b_\ell - 1) + 1$. The function h_ℓ maps B_ℓ injectively into a table of size m_ℓ. We arrange the subtables into a single table. Then the subtable for B_ℓ starts at position $s_\ell = m_0 + \ldots + m_{\ell-1}$ and ends at position $s_\ell + m_\ell - 1$.

Lemma 11. $\mathrm{E}[C(h)] \leq cn(n-1)/m$. *Also, for at least half of the functions $h \in H_m$, we have $C(h) \leq 2cn(n-1)/m$.*

Proof. We define $n(n-1)$ indicator random variables $X_{ij}(h)$. For $i \neq j$, let $X_{ij}(h) = 1$ iff $h(k_i) = h(k_j)$. Then $C(h) = \sum_{ij} X_{ij}(h)$ and hence

$$\mathrm{E}[C] = \mathrm{E}[\sum_{ij} X_{ij}] = \sum_{ij} \mathrm{E}[X_{ij}] = \sum_{ij} \mathrm{prob}(X_{ij} = 1) \leq n(n-1) \cdot c/m\ ,$$

where the second equality follows from linearity of expectations (see Equation (A.2)) and the last equality follows from universality of H_m. The second claim follows from Chebychev's inequality (A.4).

If we are willing to work with a quadratic size table, our problem is solved.

Lemma 12. *If $m \geq cn(n-1) + 1$, at least half the functions $h \in H_m$ operate injectively on S.*

Proof. By Lemma 11, we have $C(h) < 2$ for half of the functions in H_m. Since $C(h)$ is even, $C(h) < 2$ implies $C(h) = 0$ and so h operates injectively on S.

So we choose a random $h \in H_m$ with $m \geq cn(n-1) + 1$ and check whether it is injective on S. If not, we repeat the exercise. After an average of two trials, we are successful.

In the remainder of the section, we show how to bring the table size down to linear. The idea is to use a two-stage mapping of keys, see Figure 4.3. The first stage maps keys to buckets of constant average size. The second stage spends a quadratic amount of space for each bucket. We will use the information about $C(h)$ to bound the number of keys hashing to any table location. For $\ell \in [0..m-1]$ and $h \in H_m$, let B_ℓ^h be the elements in S that are mapped to ℓ by h and let b_ℓ^h be the cardinality of B_ℓ^h.

Lemma 13. $C(h) = \sum_\ell b_\ell^h(b_\ell^h - 1)$.

Proof. For any ℓ, the keys in B_ℓ^h give rise to $b_\ell^h(b_\ell^h - 1)$ pairs of keys mapping to the same location. Summation over ℓ completes the proof.

The construction of the perfect hash function is now as follows. Let α be a constant which we fix later. We choose a hash function $h \in H_{\lceil \alpha n \rceil}$ to split S into subsets B_ℓ. Of course, we choose h in the good half of $H_{\lceil \alpha n \rceil}$, i.e., we choose $h \in H_{\lceil \alpha n \rceil}$ with $C(h) \leq 2cn(n-1)/\lceil \alpha n \rceil \leq 2cn/\alpha$. For each ℓ, let B_ℓ be the elements in S mapped to ℓ and let $b_\ell = |B_\ell|$.

Consider now any B_ℓ. Let $m_\ell = cb_\ell(b_\ell - 1) + 1$. We choose a function $h_\ell \in H_{m_\ell}$ which maps B_ℓ injectively into $[0..m_\ell - 1]$. Half of the functions in H_{m_ℓ} have this property by Lemma 12 applied to B_ℓ. In other words, h_ℓ maps B_ℓ injectively into a table of size m_ℓ. We stack the various tables on top of each other to obtain one large table of size $\sum_\ell m_\ell$. In this large table, the subtable for B_ℓ starts at position $s_\ell = m_0 + m_1 + \ldots + m_{\ell-1}$. Then

$$\ell := h(x).\ \text{Return } s_\ell + h_\ell(x)$$

computes an injective function on S. The function values are bounded by

$$\begin{aligned}\sum_\ell m_\ell &\leq \lceil \alpha n \rceil + c \cdot \sum_\ell b_\ell(b_\ell - 1)\\ &\leq 1 + \alpha n + c \cdot C(h)\\ &\leq 1 + \alpha n + c \cdot 2cn/\alpha\\ &\leq 1 + (\alpha + 2c^2/\alpha)n\end{aligned}$$

and hence we have constructed a perfect hash function mapping S into a linearly sized range, namely $[0..(\alpha + 2c^2/\alpha)n]$. In the derivation above, the first inequality uses the definition of the m_ℓ's, the second inequality uses Lemma **??**, and the third inequality uses $C(h) \leq 2cn/\alpha$. The choice $\alpha = \sqrt{2}c$ minimizes the size of the range. For $c = 1$, the size of the range is $2\sqrt{2}n$.

Theorem 13. *For any set of n keys, a perfect hash function with range $[0..2\sqrt{2}n]$ can be constructed in linear expected time.*

Constructions with smaller ranges are known. Also, it is possible to support insertions and deletions.

Exercise 66 (Dynamization:). We will outline a scheme for dynamization. Consider a fixed S and choose $h \in H_{2\lceil \alpha n \rceil}$. For any ℓ let $m_\ell = 2cb_\ell(b_\ell - 1) + 1$, i.e., all m's are chosen twice as large as in the static scheme. Construct a perfect hash function as above. Insertion of a new x is handled as follows. Assume h maps x onto ℓ. If h_ℓ is no longer injective, choose a new h_ℓ. If b_ℓ becomes so large that $m_\ell = cb_\ell(b_\ell - 1) + 1$, choose a new h.

4.6 Implementation Notes

Although hashing is an algorithmically simple concept, a clean, efficient, and robust implementation can be surprisingly nontrivial. Less surprisingly, the most important issue are hash functions. Most applications seem to use simple very fast hash functions based on `xor`, shifting, and table lookups rather than universal hash functions, see for example `www.burtleburtle.net/bob/hash/doobs.html` or search for "hash table" in the internet. Although these functions seem to work well in practice, we believe that the universal hash functions presented in Section 4.2 are competitive. Unfortunately, there is no implementation study. In particular, family $H^{\oplus[]}$ from Exercise 63 should be suitable for integer keys and Exercise 56 formulates a good function for strings. It might be possible to implement the latter function particularly fast using the *SIMD-instructions* in modern processors that allow the parallel execution of several small precision operations.

Implementing Hashing with Chaining:

Hashing with chaining uses only very specialized operations on sequences, for which singly linked lists are ideally suited. Since these lists are extremely short, some deviations from the implementation scheme from Section 3.1 are in order. In particular, it would be wasteful to store a dummy item with each list. Instead, one should use a single shared dummy item to mark the end of all lists. This item can then be used as a sentinel element for *find* and *remove* as in function *findNext* in Section 3.1.1. This trick not only saves space, but also makes it likely that the dummy item resides in the cache memory.

With respect to the first element of the lists there are two alternatives. One can either use a table of pointers and store the first element outside the table or store the first element of each list directly in the table. We refer to the alternatives as *slim tables* and *fat tables*, respectively. Fat tables are usually faster and more space efficient. Slim tables are superior when elements are very large. Observe that a slim table wastes the space for m pointers and that a fat table wastes the space of the unoccupied table positions, see Exercise 54. Slim tables also have the advantage of referential integrity even when tables are reallocated. We have already observed this complication for unbounded arrays in Section 3.6.

Comparing the space consumption of hashing with chaining and linear probing is even more subtle than outlined in Section 4.4. On the one hand, the linked lists burden the memory management with many small pieces of allocated memory. See Section 3.1.1 for a discussion of memory management for linked lists. On the other hand, implementations of unbounded hash tables based on chaining can avoid occupying two tables during reallocation by using the following method: first, concatenate all lists to a single list L. Deallocate the old table. Only then allocate the new table. Finally, scan L moving the elements to the new table.

Exercise 67. Implement hashing with chaining and linear probing on your own machine using your favorite programming language. Make experiments to compare their performance. Also try hash table implementations from software libraries in comparison. Use elements of size 8 byte.

Exercise 68 (Large elements.). Repeat the measurements with element sizes 32 and 128. Also, add an implementation of *slim chaining*, where table entries only store pointers to the first list element (see also Section 4.6 below).

Exercise 69 (Large keys). Discuss the impact of large keys on the relative merits of chaining versus linear probing. Which variant will profit? Why?

Exercise 70. Implement a hash table data type for very large tables stored in a file. Should you use chaining or linear probing? Why?

C++:

The C++ standard library does not define a hash table data type. However, the popular implementation by SGI (`http://www.sgi.com/tech/stl/`) offers several variants: $hash\_set$, $hash\_map$, $hash\_multiset$, $hash\_multimap$. Here "set" stands for the kind of interfaces used in this chapter whereas a "map" is an associative array indexed by Keys. The term "multi" stands for data types that allow multiple elements with the same key. Hash functions are implemented as *function objects*, i.e., the class `hash<T>` overloads the operator "`()`" so that an object can be used like a function. The reason for this approach is that it allows the hash function to store internal state such as random coefficients.

LEDA offers several hashing based implementations of dictionaries. The class $h\_array\langle Key, T\rangle$ implements an associative array storing objects of type T assuming that a hash function $int\ Hash(Key\&)$ is defined by the user and returns an integer value that is then mapped to a table index by LEDA. The implementation uses hashing with chaining and adapts the table size to the number of elements stored. The class map is similar but uses a built-in hash function.

Java:

The class $java.util.hashtable$ implements unbounded hash tables using the function $hashCode$ defined in class $Object$ as a hash function.

Exercise 71 (Associative arrays.). Implement a C++-class for associative arrays. Support `operator[]` for any index type that supports a hash function. Make sure that `H[x]=...` works as expected if x is the key of a new element.

4.7 Historical Notes and Further Findings

Hashing with chaining and hashing with linear probing was already used in the fifties. The analysis of hashing began soon after. In the 60s and 70s, average case analysis in the spirit of Theorem 10 prevailed. Different schemes were analysed for random sets of keys and random hash functions. An early survey paper was written by Morris [136]. The book [109] contains a wealth of material.[todo:some theoretical results for linear probing] ⟹

Universal hash functions were introduced by Carter and Wegman [35]. The original paper proves Theorem 11 und introduces the universal classes discussed in Exercises 59. [Who introduced the other classes] ⟹ The family in Exercise 62 is due to Keller and Abholhassan. Perfect hashing was a black art till Fredman, Komlos, and

Szemeredi [65] introduced the construction shown in Theorem 13. Dynamization is due to M. Dietzfelbinger, A. Karlin, K. Mehlhorn, F. Meyer auf der Heide, H. Rohnert, and R. Tarjan [55]. Cuckoo Hashing [145] is an alternative approach to perfect hashing.

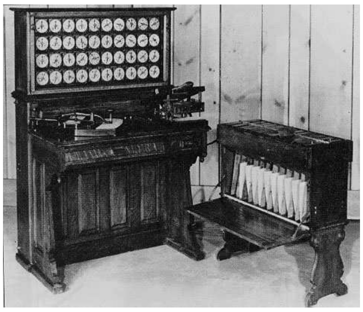
Universal hashing bounds the probability of any two keys colliding. A more general notion is k-way independence; here k is a positive integer. A family H of hash functions is *k-way independent* if for some constant c, any k distinct keys x_1 to x_k and any k hash values a_1 to a_k, $\mathrm{prob}(h(x_1) = a_1 \wedge \cdots \wedge h(x_k) = a_k) \leq c/m^k$. A simple k-wise independent family of hash functions are polynomials of degree $k-1$ with random coefficients [34], see Exercise 60.

The *maximum occupancy* is the maximal number of elements hashed to the same position, i.e., $\max_\ell b_\ell^h$. Assume $n = m$. A random hash function produces an expected maximum occupancy of $\mathcal{O}(\log m / \log\log m)$. Universal families produce expected maximum occupancy $\mathcal{O}(\sqrt{n})$; this follows from Lemmas 11 and 13. k-wise independent hash functions guarantee maximum expected occupancy $\mathcal{O}\left(n^{1/k}\right)$, see [55]. Maximum occupancy is relevant in real time and parallel environments. Dietzfelbinger and Meyer auf der Heide [56][check ref] give a family of hash functions that [which bound, outline trick.]. [m vs n dependence?] ⟸ ⟸

[todo: some remarks on cryptographic hash functions] ⟸ ⟸

5

Sorting and Selection



Telephone directories are sorted alphabetically by last names. Why? Because a sorted index can be searched quickly. Even in the telephone directory of a huge city one can usually find a name in a few seconds. In an unsorted index, nobody would even try to find a name. In a first approximation, this chapter teaches you how to turn an unordered collection of elements into an ordered collection, i.e., how to sort *the collection. However, sorting has many other uses as well. An early example of a massive data processing task is the statistical evaluation of census data. 1500 people needed seven years to manually process the US census in 1880. The engineer Herman Hollerith*[1]*, who participated in this evaluation as a statistician, spent much of the ten years to the next census developing counting and sorting machines for mechanizing this gigantic endeavor. Although the 1890 census had to evaluate more people and more questions, the basic evaluation was finished in 1891. Hollerith's company continued to play an important role in the development of the information processing industry; since 1924 it has been known as International Business Machines (IBM). Sorting is important for census statistics because one often wants to form subcollections, e.g., all persons between age 20 and 30 and living on a farm. Two applications of sorting solve the problem. First sort all persons by age and form the subcollection*

[1] The picuture to the right shows Herman Hollerith, born February 29 1860, Buffalo NY; died November 17, 1929, Washington DC. The small machine in the picture on the left is one of his sorting machines.

of persons between 20 and 30 years of age. Then sort the subcollection by home and extract the subcollection of persons living on a farm.

Although we probably all have an intuitive concept of what *sorting* is about, let us give a formal definition. The input is a sequence $s = \langle e_1, \ldots, e_n \rangle$ of n elements. Each element e_i has an associated *key* $k_i = \mathit{key}(e_i)$. The keys come from an ordered universe, i.e., there is a linear order $\leq$ defined on keys[2]. For ease of notation, we extend the comparison relation to elements so that $e \leq e'$ if and only if $\mathit{key}(e) \leq \mathit{key}(e')$. The task is to produce a sequence $s' = \langle e'_1, \ldots, e'_n \rangle$ such that s' is a permutation of s and such that $e'_1 \leq e'_2 \leq \cdots \leq e'_n$. Observe that the ordering of equivalent elements is arbitrary.

Although different comparison relations for the same data type may make sense, the most frequent relations are the obvious order for numbers and the *lexicographic order* (see Appendix A) for tuples, strings, or sequences. The lexicographic order for strings comes in different flavors. We may declare the same small and capital characters as equivalent or not and different rules for treating accented characters are used in different contexts.

Exercise 72. Given linear orders $\leq_A$ of A and $\leq_B$ of B define a linear order on $A \times B$.

Exercise 73. Define a total order for complex numbers where $x \leq y$ implies $|x| \leq |y|$.

Sorting is an ubiquitous algorithmic tool; it is frequently used as a preprocessing step in more complex algorithms. We will give some examples.

Preprocessing for fast search: In Section 2.5 on binary search, we have already seen that not only humans can search a sorted directory more easily than an unsorted one. Moreover a sorted directory supports additional operations such as finding all elements in a certain range. We will discuss searching in more detail in Chapter 7. Hashing is a method for searching unordered sets.

Grouping: Often we want to bring equal elements together to count them, eliminate duplicates, or otherwise process them. Again, hashing is an alternative. But sorting has advantages since we will see rather fast deterministic algorithms for it that use very little space and that extend gracefully to huge data sets.

Processing in sorted order: Certain algorithms become very simple if the inputs are processed in sorted order. Exercise 74 gives an example. Other examples are Kruskal's algorithm in Section 11.3 and several of the algorithms for the knapsack problem in Chapter 12. You may also want to remember sorting when you solve Exercise 154 on interval graphs.

[2] A linear order is a reflexive, transitive and weakly antisymmetric relation $\leq$, i.e., $x \leq x$ for all x, $x \leq y$ and $y \leq z$ imply $x \leq z$, and for any two x and y either $x \leq y$ or $y \leq x$ or both. Two keys x and y are called equivalent if $x \leq y$ and $y \leq x$; we write $x \equiv y$. If $x \not\equiv y$, exactly one of $x \leq y$ or $y \leq x$ holds. We write $x < y$ in the former case and $y < x$ in the latter case.

In Section 5.1 we will introduce several simple sorting algorithms. They have quadratic complexity, but are still useful for small input sizes. Moreover, we will learn some low-level optimizations. Section 5.2 introduces *mergesort*, a simple divide-and-conquer sorting algorithm that runs in time $\mathcal{O}(n \log n)$. Section 5.3 establishes that this bound is optimal for all *comparison-based* algorithms, i.e., algorithms that treat elements as black boxes that can only be compared and moved around. The quicksort algorithm described in Section 5.4 is also based on the divide-and-conquer principle and is perhaps the most frequently used sorting algorithm. Quicksort is also a good example for a randomized algorithm. The idea behind quicksort leads to a simple algorithm for a problem related to sorting. Section 5.5 explains how the k-th smallest from n elements can be found in time $\mathcal{O}(n)$. Sorting can be made even faster than the lower bound from Section 5.3 by looking at the bit pattern of the keys as explained in Section 5.6. Finally, Section 5.7 generalizes quicksort and mergesort to very good algorithms for sorting inputs that do not fit into internal memory.

Exercise 74 (A simple scheduling problem). A hotel manager has to process n advance bookings of rooms for the next season. His hotel has k identical rooms. Bookings contain arrival date and departure date. He wants to find out whether there are enough rooms in the hotel to satisfy the demand. Design an algorithm that solves this problem in time $\mathcal{O}(n \log n)$. Hint: Consider the set of all arrivals and departures. Sort the set and process in sorted order.

Exercise 75 (Sorting with few different keys). Design an algorithm that sorts n elements in $\mathcal{O}(k \log k + n)$ expected time if there are only k different keys appearing in the input. Hint: Combine hashing and sorting.

Exercise 76 (Checking). It is easy to check whether a sorting routine produces sorted output. It is less easy to check whether the output is also a permutation of the input. But here is a fast and simple Monte Carlo algorithm for integers: (1) Show that $\langle e_1, \ldots, e_n \rangle$ is a permutation of $\langle e'_1, \ldots, e'_n \rangle$ iff the polynomial $q(z) := (z - e_1) \cdots (z - e_n) - (z - e'_1) \cdots (z - e'_n)$ is identically zero. Here z is a variable. (2) For any $\epsilon > 0$ let p be a prime with $p > \max \{n/\epsilon, e_1, \ldots, e_n, e'_1, \ldots, e'_n\}$. Now the idea is to evaluate the above polynomial $\bmod p$ for a random value $z \in [0..p-1]$. Show that if $\langle e_1, \ldots, e_n \rangle$ is *not* a permutation of $\langle e'_1, \ldots, e'_n \rangle$ then the result of the evaluation is zero with probability at most ϵ. Hint: A nonzero polynomial of degree n has at most n zeroes.

5.1 Simple Sorters

We will introduce two simple sorting techniques: *selection sort* and *insertion sort*.

Selection sort repeatedly selects the smallest element from the input sequence, deletes it, and adds it to the end of the output sequence. The output sequence is initially empty. The process continues until the input sequence is exhausted. For example,

$$\langle\rangle, \langle 4,7,1,1\rangle \rightsquigarrow \langle 1\rangle, \langle 4,7,1\rangle \rightsquigarrow \langle 1,1\rangle, \langle 4,7\rangle \rightsquigarrow \langle 1,1,4\rangle, \langle 7\rangle \rightsquigarrow \langle 1,1,4,7\rangle, \langle\rangle \ .$$

The algorithm can be implemented so that it uses a single array of n elements and works *in place*, i.e., needs no additional storage beyond the input array and a constant amount of space for loop counters etc. The running time is quadratic.

Exercise 77 (Simple selection sort). Implement selection sort so that it sorts an array with n elements in time $\mathcal{O}(n^2)$ by repeatedly scanning the input sequence. The algorithm should be in-place, i.e., both the input sequence and the output sequence should share the same array. Hint: The implementation operates in n phases numbered 1 to n. At the beginning of the i-th phase, the first $i-1$ locations of the array contain the $i-1$ smallest elements in sorted order and the remaining $n-i+1$ locations contain the remaining elements in arbitrary order.

In Section 6.5 we will learn about a more sophisticated implementation where the input sequence is maintained as a *priority queue*. Priority queues support efficient repeated selection of the minimum element. The resulting algorithm runs in time $\mathcal{O}(n \log n)$ and is frequently used. It is efficient, it is deterministic, it works in-place, and the input sequence can be dynamically extended by elements that are larger than all previously selected elements. The last feature is important in discrete event simulations where events are to be processed in increasing order of time and processing an event may generate further events in the future.

Selection sort maintains the invariant that the output sequence is sorted by carefully choosing the element to be deleted from the input sequence. *Insertion sort* maintains the same invariant by choosing an arbitrary element of the input sequence but taking care to insert this element at the right place in the output sequence. For example,

$$\langle\rangle, \langle 4,7,1,1\rangle \rightsquigarrow \langle 4\rangle, \langle 7,1,1\rangle \rightsquigarrow \langle 4,7\rangle, \langle 1,1\rangle \rightsquigarrow \langle 1,4,7\rangle, \langle 1\rangle \rightsquigarrow \langle 1,1,4,7\rangle, \langle\rangle \ .$$

Figure 5.1 gives an in-place array implementation of insertion sort. The implementation is straightforward except for a small trick that allows the inner loop to use only a single comparison. When the element e to be inserted is smaller than all previously inserted elements, it can be inserted at the beginning without further tests. Otherwise, it suffices to scan the sorted part of a from right to left while e is smaller than the current element. This process has to stop because $a[1] \leq e$. In the worst case, insertion sort is quite slow. For example, if the input is sorted in decreasing order, each input element is moved all the way to $a[1]$, i.e., in iteration i of the outer loop, i elements have to be moved. Overall, we obtain

$$\sum_{i=2}^{n}(i-1) = -n + \sum_{i=1}^{n} i = \frac{n(n+1)}{2} - n = \frac{n(n-1)}{2} = \Omega(n^2)$$

movements of elements (see also Equation (A.11)).

Nevertheless, insertion sort is useful. It is fast for small inputs (say $n \leq 10$) and hence can be used as the base case in divide-and-conquer algorithms for sorting. Furthermore, in some applications the input is already "almost" sorted and in this situation insertion sort will be fast.

```
Procedure insertionSort($a$ : Array $[1..n]$ of Element)
    for $i := 2$ to $n$ do
        invariant $a[1] \le \cdots \le a[i-1]$
        // move $a[i]$ to the right place
        $e := a[i]$
        if $e < a[1]$ then                                              // new minimum
            for $j := i$ downto $2$ do $a[j] := a[j-1]$
            $a[1] := e$
        else                                                   // use $a[1]$ as a sentinel
            for $j := i$ downto $-\infty$ while $a[j-1] > e$ do $a[j] := a[j-1]$
            $a[j] := e$
```

Fig. 5.1. Insertion sort

Exercise 78 (Almost sorted inputs). Prove that insertion sort runs in time $\mathcal{O}(n + D)$ where $D = \sum_i |r(e_i) - i|$ and $r(e_i)$ is the *rank* (position) of e_i in the sorted output.

Exercise 79 (Average case analysis). Assume that the input to insertion sort is a permutation of the numbers 1 to n. Show that the average execution time over all possible permutations is $\Omega(n^2)$. Hint: Argue formally that about one third of the input elements in the right third of the array have to be moved to the left third of the array. Can you improve the argument to show that on average $n^2/4 - \mathcal{O}(n)$ iterations of the inner loop are needed?

Exercise 80 (Insertion sort with few comparisons). Modify the inner loops of the array-based insertion sort algorithm from Figure 5.1 so that it needs only $\mathcal{O}(n \log n)$ comparisons between elements. Hint: Use binary search as discussed in Chapter 7. What is the running time of this modification of insertion sort?

Exercise 81 (Efficient insertion sort?). Use the data structure for sorted sequences from Chapter 7 to derive a variant of insertion sort that runs in time $\mathcal{O}(n \log n)$. How will this sorting algorithm compare to mergesort or quicksort?

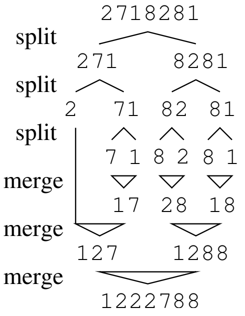
***Exercise 82 (Formal verification)** Use your favorite verification formalism, e.g. Hoare calculus, to prove that insertion sort produces a permutation of the input (produces a sorted permutation of the input).

5.2 Mergesort — an $\mathcal{O}(n \log n)$ Sorting Algorithm

Mergesort is a straightforward application of the divide-and-conquer principle. The unsorted sequence is split into two parts of about equal size. The parts are sorted recursively and the sorted parts are merged into a single sorted sequence. The approach is efficient because merging two sorted sequences a and b is quite simple. The globally smallest element is either the first element of a or the first element of b. So we move the smaller element to the output, find the second smallest element

```
**Function** mergeSort($\langle e_1,\ldots,e_n\rangle$) : Sequence **of** Element
    **if** $n = 1$ **then return** $\langle e_1\rangle$
    **else return** $merge(mergeSort(e_1,\ldots,e_{\lfloor n/2\rfloor}), mergeSort(e_{\lfloor n/2\rfloor+1},\ldots,e_n))$

// merging two sequences represented as lists
**Function** merge($a, b$ : Sequence **of** Element) : Sequence **of** Element
    $c := \langle\rangle$
    **loop**
        **invariant** $a$, $b$, and $c$ are sorted and $\forall e \in c, e' \in a \cup b : e \le e'$
        **if** $a.isEmpty$              **then**  $c.concat(b)$; **return** $c$
        **if** $b.isEmpty$              **then**  $c.concat(a)$; **return** $c$
        **if** $a.first \le b.first$ **then**  $c.moveToBack(a.first)$
        **else**                                  $c.moveToBack(b.first)$
```

Fig. 5.2. Mergesort



a	b	c	operation
$\langle 1,2,7\rangle$	$\langle 1,2,8,8\rangle$	$\langle\rangle$	move a
$\langle 2,7\rangle$	$\langle 1,2,8,8\rangle$	$\langle 1\rangle$	move b
$\langle 2,7\rangle$	$\langle 2,8,8\rangle$	$\langle 1,1\rangle$	move a
$\langle 7\rangle$	$\langle 2,8,8\rangle$	$\langle 1,1,2\rangle$	move b
$\langle 7\rangle$	$\langle 8,8\rangle$	$\langle 1,1,2,2\rangle$	move a
$\langle\rangle$	$\langle 8,8\rangle$	$\langle 1,1,2,2,7\rangle$	move a
$\langle\rangle$	$\langle\rangle$	$\langle 1,1,2,2,7,8,8\rangle$	concat b

Fig. 5.3. Execution of $mergeSort(\langle 2,7,1,8,2,8,1\rangle)$. The left part illustrates the recursion in $mergeSort$ and the right part illustrates the $merge$ in the outermost call.

using the same approach and iterate until all elements have been moved to the output. Figure 5.2 gives pseudocode and Figure 5.3 illustrates a sample execution. We have elaborated the merging routine for sequences represented as linear lists as introduced in Section 3.1. Note that no allocation and deallocation of list items is needed. Each iteration of the inner loop of $merge$ performs one element comparison and moves one element to the output. Each iteration takes constant time. Hence merging runs in linear time.

Theorem 14. *Function* $merge$ *applied to sequences of total length* n *executes in time* $\mathcal{O}(n)$ *and performs at most* $n-1$ *element comparisons.*

For the running time of mergesort we obtain.

Theorem 15. *Mergesort runs in time* $\mathcal{O}(n\log n)$ *and performs no more than* $n\log n$ *element comparisons.*

Proof. Let $C(n)$ denote the worst case number of element comparisons performed. We have $C(1) = 0$ and $C(n) \le C(\lfloor n/2\rfloor) + C(\lceil n/2\rceil) + n - 1$ using Theorem 14.

The master theorem for recurrence relations (6) suggests that $C(n) = \mathcal{O}(n \log n)$. We give two proofs. The first proof shows $C(n) \le 2n \lceil \log n \rceil$ and the second proof shows $C(n) \le n \lceil \log n \rceil$.

For n a power of two, define $D(1) = 0$ and $D(n) = 2D(n/2) + n$. Then $D(n) = n \log n$ for n a power of two by the master theorem for recurrence relations. We claim that $C(n) \le D(2^k)$ where k is such that $2^{k-1} < n \le 2^k$. Then $C(n) \le D(2^k) = 2^k k \le 2n \lceil \log n \rceil$. It remains to argue the inequality $C(n) \le D(2^k)$. We use induction on k. For $k = 0$, we have $n = 1$ and $C(1) = 0 = D(1)$ and the claim certainly holds. For $k > 1$, we observe that $\lfloor n/2 \rfloor \le \lceil n/2 \rceil \le 2^{k-1}$ and hence

$$C(n) \le C(\lfloor n/2 \rfloor) + C(\lceil n/2 \rceil) + n - 1 \le 2D(2^{k-1}) + 2^k - 1 \le D(2^k) .$$

This completes the first proof. We turn to the refined proof. We prove that

$$C(n) \le n \lceil \log n \rceil - 2^{\lceil \log n \rceil} + 1 \le n \log n$$

by induction over n. For $n = 1$, the claim is certainly true. So assume $n > 1$. We distinquish two cases. Assume first that we have $2^{k-1} < \lfloor n/2 \rfloor \le \lceil n/2 \rceil \le 2^k$ for some integer k. Then $\lceil \log \lfloor n/2 \rfloor \rceil = \lceil \log \lceil n/2 \rceil \rceil = k$ and $\lceil \log n \rceil = k + 1$ and hence

$$\begin{aligned}
C(n) &\le C(\lfloor n/2 \rfloor) + C(\lceil n/2 \rceil) + n - 1 \\
&\le \big(\lfloor n/2 \rfloor k - 2^k + 1 \big) + \big(\lceil n/2 \rceil k - 2^k + 1 \big) + n - 1 \\
&= nk + n - 2^{k+1} + 1 = n(k+1) - 2^{k+1} + 1 = n \lceil \log n \rceil - 2^{\lceil \log n \rceil} + 1 .
\end{aligned}$$

Otherwise, we have $\lfloor n/2 \rfloor = 2^{k-1}$ and $\lceil n/2 \rceil = 2^{k-1} + 1$ for some integer k and therefore $\lceil \log \lfloor n/2 \rfloor \rceil = k - 1$, $\lceil \log \lceil n/2 \rceil \rceil = k$ and $\lceil \log n \rceil = k + 1$. Thus

$$\begin{aligned}
C(n) &\le C(\lfloor n/2 \rfloor) + C(\lceil n/2 \rceil) + n - 1 \\
&\le \big(2^{k-1}(k-1) - 2^{k-1} + 1 \big) + \big((2^{k-1} + 1)k - 2^k + 1 \big) + 2^k + 1 - 1 \\
&= (2^k + 1)k - 2^{k-1} - 2^{k-1} + 1 + 1 \\
&= (2^k + 1)(k+1) - 2^{k+1} + 1 = n \lceil \log n \rceil - 2^{\lceil \log n \rceil} + 1 .
\end{aligned}$$

The bound for the execution time can be verified using a similar recurrence relation.

Mergesort is the method of choice for sorting linked lists and is therefore frequently used in functional and logical programming languages that have lists as their primary data structure. In Section 5.3 we will see that mergesort is basically optimal as far as the number of comparisons is concerned; so it is also a good choice if comparisons are expensive. When implemented using arrays, mergesort has the additional advantage that it streams through memory in a sequential way. This makes it efficient in memory hierarchies. Section 5.7 has more on that issue. Mergesort is still not the usual method of choice for an efficient array-based implementation since *merge* does not work in-place. (But see Exercise 88 for a possible way out.)

Exercise 83. Explain how to insert k new elements into a sorted list of size n in time $\mathcal{O}(k \log k + n)$.

Exercise 84. We discussed *merge* for lists but used abstract sequences for the description of *mergeSort*. Give the details of *mergeSort* for linked lists.

Exercise 85. Implement mergesort in your favorite functional programming language.

Exercise 86. Give an efficient array-based implementation of mergesort in your favorite imperative programming language. Besides the input array, allocate one auxiliary array of size n at the beginning and then use these two arrays to store all intermediate results. Can you improve running time by switching to insertion sort for small inputs? If so, what is the optimal switching point in your implementation?

Exercise 87. The way we describe *merge*, there are three comparisons for each loop iteration — one element comparison and two termination tests. Develop a variant using sentinels that needs only one termination test. Can you do it without appending dummy elements to the sequences?

Exercise 88. Exercise 47 introduces a list-of-blocks representation for sequences. Implement merging and mergesort for this data structure. In merging, reuse emptied input blocks for the output sequence. Compare space and time efficiency of mergesort for this data structure, plain linked lists, and arrays. Pay attention to constant factors.

5.3 A Lower Bound

Algorithms give upper bounds on the complexity of a problem. By the preceding discussion we know that we can sort n items in time $\mathcal{O}(n \log n)$. Can we do better, maybe even achieve linear time? A "yes" answer requires a better algorithm and its analysis. But how could be potentially argue a "no" answer? We would have to argue that no algorithm, however ingenious, can run in time $o(n \log n)$. Such an argument is called a *lower bound*. So what is the answer? The answer is no and yes. The answer is no, if we restrict ourselves to comparison-based algorithms and the answer is yes, if we go beyond comparison-based algorithms. We will discuss non-comparison-based sorting in Section 5.6.

So what is a comparison-based sorting algorithm? The only way, it can learn
⟹ about its inputs is by comparing two input elements[ps was: them]. It is not allowed
⟹ to exploit the representation of keys as bitstrings. [ps inserted word] Deterministic comparison-based algorithms can be viewed as trees. We make an initial comparison, say the algorithms asks "$e_i \leq e_j$?" with outcomes yes and no. Based on the outcome, the algorithm proceeds to the next comparison. The key point is that the comparison made next depends only on the outcome of all preceding comparisons and nothing else. Figure 5.4 shows a sorting tree for three elements.

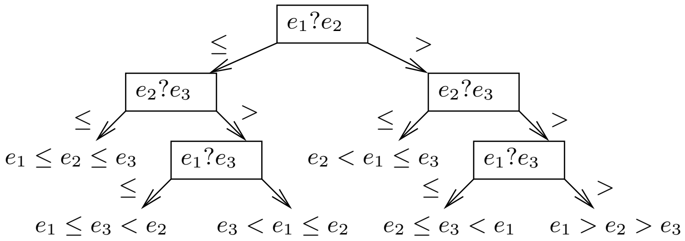


Fig. 5.4. A tree that sorts three elements. We first compare e_1 and e_2. If $e_1 \leq e_2$, we compare e_3 with e_2. If $e_2 \leq e_3$, we have $e_1 \leq e_2 \leq e_3$ and are finished. Otherwise, we compare e_1 with e_3. For either outcome, we are finished. If $e_1 > e_2$, we compare e_2 with e_3. If $e_2 > e_3$, we have $e_1 > e_2 > e_3$ and are finished. Otherwise, we compare e_1 with e_3. For either outcome, we are finished. The worst-case number of comparisons is three. The average number is $(2+3+3+2+3+3)/6 = 8/3$.

When the algorithms terminates, it must have collected sufficient information so that it can commit to a permutation of the input. When can it commit? We perform the following thought experiment. We assume that the input keys are distinct and we consider any of the $n!$ permutations of the inputs, say π. The permutation π corresponds to the situation that $e_{\pi(1)} < e_{\pi(2)} < \ldots < e_{\pi(n)}$. We answer all questions posed by the algorithm so that they conform to the ordering defined by π. This will lead us to a leaf ℓ_π of the comparison tree.

Lemma 14. *Let π and σ be two distinct permutations of n elements. Then the leaves ℓ_π and ℓ_σ must be distinct.*

Proof. Assume otherwise. In the leaf, the algorithm commits to some ordering of the input and so it cannot commit to both π and σ. Say it commits to π. Then, on an input ordered according to σ, the algorithm is incorrect, a contradiction.

The lemma above tells us that any comparison tree for sorting must have at least $n!$ leaves. Since a tree of depth T has at most 2^T leaves, we must have

$$2^T \geq n! \quad \text{or} \quad T \geq \log n! \ .$$

Via Stirling's approximation of the factorial (Equation (A.9)) we obtain:

$$T \geq \log n! \geq \log \left(\frac{n}{e}\right)^n = n \log n - n \log e \ .$$

Theorem 16. *Any comparison-based sorting algorithm needs $n \log n - \mathcal{O}(n)$ comparisons in the worst case.*

We state without proof that the bound also applies to randomized sorting algorithms and to to the average case complexity of sorting, i.e., worst case sorting problems are not much more difficult than randomly permuted inputs. Furthermore, the bound even applies if we only want to solve the seemingly simpler problem of checking whether some element appears twice in a sequence.

Theorem 17. *Any comparison-based sorting algorithm needs $n \log n - \mathcal{O}(n)$ comparisons on average, i.e,*

$$\frac{\sum_\pi d_\pi}{n!} = n \log n - \mathcal{O}(n) \ ,$$

where the sum extends over all $n!$ permutations of n elements and d_π is the depth of leaf ℓ_π.

Exercise 89. Show that any comparison-based algorithm for determining the smallest among n elements requires $n - 1$ comparisons. Also show that any comparison-based algorithm for determining the smallest and the second smallest elements among n elements requires at least $n - 1 + \log n$ comparisons. Give an algorithm with this performance.

Exercise 90. The *element uniqueness problem* is the task of deciding whether in a $\Longrightarrow$ set of n elements[ps added comma], all elements are pairwise distinct. Argue that comparison-based algorithms require $\Omega(n \log n)$ comparisons. Why does this not contradict the fact, that with we can solve the problem in linear expected time using hashing?

Exercise 91 (Lower bound for average case). With the notation above let d_π be the depth of the leaf ℓ_π. Argue that $A = (1/n!) \sum_\pi d_\pi$ is the average case complexity of a comparison-based sorting algorithm. Try to show $A \geq \log n!$. Hint: prove first that $\sum_\pi 2^{-d_\pi} \leq 1$. Then consider the minimization problem "minimize $\sum_\pi d_\pi$ subject to $\sum_\pi 2^{-d_\pi} \leq 1$". Argue that the minimum is attained when all d_i are equal.

Exercise 92 (Sorting small inputs optimally). Give an algorithm for sorting k element using at most $\lceil \log k! \rceil$ element comparisons: (a) for $k \in \{2, 3, 4\}$ use mergesort. (b) for $k = 5$ you are allowed to use 7 comparisons. This is difficult. Mergesort does not do the job as it uses up to 8 comparisons. (c) for $k \in \{6, 7, 8\}$ use the case $k = 5$ as a subroutine.

5.4 Quicksort

Quicksort is a divide-and-conquer algorithm that is complementary to the mergesort algorithm of Section 5.2. Quicksort does all the difficult work *before* the recursive calls. The idea is to distribute the input elements to two or more sequences that $\Longrightarrow$ represent nonoverlapping[ps was: disjoint] ranges of key values. Then it suffices to sort the shorter sequences recursively and to concatenate the results. To make the duality to mergesort complete, we would like to split the input into two sequences of equal size. Unfortunately, this is a non-trivial task. However, we can come close by picking a random splitter element. The splitter element is usually called *pivot*. Let p denote the pivot element chosen. Elements are classified into three sequences a, b, and c of elements that are smaller, equal to, or larger than p respectively. Figure 5.5 gives a high-level realization of this idea and Figure 5.6 depicts a sample execution.

```
Function quickSort(s : Sequence of Element) : Sequence of Element
    if $|s| \leq 1$ then return s                                  // base case
    pick $p \in s$ uniformly at random                              // pivot key
    $a := \langle e \in s : e < p \rangle$
    $b := \langle e \in s : e = p \rangle$
    $c := \langle e \in s : e > p \rangle$
    return concatenation of quickSort(a), b, and quickSort(c)
```

Fig. 5.5. Quicksort

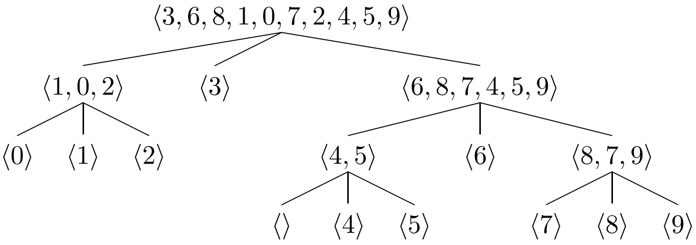


Fig. 5.6. Execution of *quickSort* (Figure 5.5) on $\langle 3,6,8,1,0,7,2,4,5,9\rangle$ using the first element of a subsequence as the pivot: The first call of quicksort uses 3 as the pivot and generates the subproblems $\langle 1,0,2\rangle$, $\langle 3\rangle$, and $\langle 6,8,7,4,5,9\rangle$. The recursive call for the third subproblem uses 6 as a pivot and generates the subproblems $\langle 4,5\rangle$, $\langle 6\rangle$, and $\langle 8,7,9\rangle$.

Quicksort has expected execution time $\mathcal{O}(n \log n)$ as we will show in Section 5.4.1. In Section 5.4.2 we discuss refinements that make quicksort the most widely used sorting algorithm in practice.

5.4.1 Analysis

To analyze the running time of quicksort for an input sequence $s = \langle e_1, \ldots, e_n \rangle$ we focus on the number of element comparisons performed. [ps moved sentence:] $\Longleftarrow$ We allow *three-way* comparisons here, with possible outcomes 'smaller', 'equal', and 'larger'. Other operations contribute only constant factors and small additive terms to the execution time.

Let $C(n)$ denote the worst case number of comparisons needed for any input sequence of size n and any choice of pivots. The worst case performance is easily determined. The subsequences a, b and c in Figure 5.5 are formed by comparing the pivot with all other elements. This makes $n-1$ comparisons. Assume there are k elements smaller than the pivot and k' elements larger than the pivot. We obtain $C(0) = C(1) = 0$ and

$$C(n) \leq n - 1 + \max\left\{C(k) + C(k') : 0 \leq k \leq n-1, 0 \leq k' < n-k\right\} .$$

By induction it is easy to verify that

$$C(n) \leq \frac{n(n-1)}{2} = \Theta\big(n^2\big) \quad .$$

The worst case occurs if all elements are different and we always pick the largest or smallest element as the pivot. Thus $C(n) = n(n-1)/2$.

The expected performance is much better. We first argue an $\mathcal{O}(n \log n)$ bound and then show a bound of $2n \ln n$. We concentrate on the case that all elements are different. Other cases are easier because a pivot that occurs several times results in a larger middle sequence b that need not be processed any further. Consider a fixed element e_i and let X_i denote the total number of times e_i is compared to a pivot element. Then $\sum_i X_i$ is the total number of comparisons. Whenever e_i is compared to a pivot element, it ends up in a smaller subproblem. Therefore $X_i \leq n-1$ and we have another proof for the quadratic upper bound. Let us call a comparison good for e_i, if e_i moves to a subproblem of at most $3/4$-th the size. Then any e_i can be involved in at most $\log_{4/3} n$ good comparisons. Also, the probability that a pivot is chosen, which is good for e_i, is at least $1/2$; this holds since a bad pivot must belong to either the smallest or largest quarter of elements. So $\mathrm{E}[X_i] \leq 2 \log_{4/3} n$ and hence $\mathrm{E}[\sum_i X_i] = \mathcal{O}(n \log n)$. We will next give a different argument and a better bound.

Theorem 18. *The expected number of comparisons performed by quicksort is*

$$\bar{C}(n) \leq 2n \ln n \leq 1.45 n \log n \quad .$$

Proof. Let $s' = \langle e'_1, \ldots, e'_n \rangle$ denote the elements of the input sequence in sorted order. Elements e'_i and e'_j are compared at most once and only if one of them is picked as a pivot. Hence, we can count comparisons by looking at the indicator random variables X_{ij}, $i < j$ where $X_{ij} = 1$ if e'_i and e'_j are compared and $X_{ij} = 0$ otherwise. We obtain

$$\bar{C}(n) = \mathrm{E}[\sum_{i=1}^{n} \sum_{j=i+1}^{n} X_{ij}] = \sum_{i=1}^{n} \sum_{j=i+1}^{n} \mathrm{E}[X_{ij}] = \sum_{i=1}^{n} \sum_{j=i+1}^{n} \mathrm{prob}(X_{ij} = 1) \quad .$$

The middle transformation follows from the linearity of expectation (Equation (A.2)). The last equation uses the definition of the expectation of an indicator random variable $\mathrm{E}[X_{ij}] = \mathrm{prob}(X_{ij} = 1)$. Before we can further simplify the expression for $\bar{C}(n)$, we need to determine the probability of X_{ij} being 1.

Lemma 15. *For any $i < j$,* $\mathrm{prob}(X_{ij} = 1) = \dfrac{2}{j - i + 1}$.

Proof. Consider the $j - i + 1$ element set $M = \{e'_i, \ldots, e'_j\}$. As long as no pivot from M is selected, e'_i and e'_j are not compared but all elements from M are passed to the same recursive calls. Eventually, a pivot p from M is selected. Each element in M has the same chance $1/|M|$ to be selected. If $p = e'_i$ or $p = e'_j$ we have $X_{ij} = 1$. The probability for this event is $2/|M| = 2/(j - i + 1)$. Otherwise, e'_i and e'_j are passed to different recursive calls so that they will never be compared.

Now we can finish proving Theorem 18 using relatively simple calculations.

$$\begin{aligned}\bar{C}(n) &= \sum_{i=1}^{n}\sum_{j=i+1}^{n} \mathrm{prob}(X_{ij}=1) = \sum_{i=1}^{n}\sum_{j=i+1}^{n} \frac{2}{j-i+1} = \sum_{i=1}^{n}\sum_{k=2}^{n-i+1} \frac{2}{k} \\ &\leq \sum_{i=1}^{n}\sum_{k=2}^{n} \frac{2}{k} = 2n\sum_{k=2}^{n}\frac{1}{k} = 2n(H_n-1) \leq 2n(1+\ln n-1) = 2n\ln n \ .\end{aligned}$$

For the last steps, recall the properties of the n-th harmonic number $H_n := \sum_{k=1}^{n} 1/k \leq 1+\ln n$ (Equation A.12).

Note that the calculations in Section 2.8 for left-right maxima were very similar although we had quite a different problem at hand.

5.4.2 Refinements

We will discuss refinements of the basic quicksort algorithm. The resulting algorithm, called $qsort$, works in place, and is fast and space efficient. Figure 5.7 shows the pseudocode and Figure 5.8 shows a sample execution. The refinements are non-trivial and we need to discuss them carefully.

Function $qsort$ operates on an array a. The arguments ℓ and r specify the subarray to be sorted. The outermost call is $qsort(a,1,n)$. If the size of the subproblem is smaller than some constant n_0, we resort to a simple algorithm[3] such as the insertion sort from Figure 5.1. The best choice for n_0 depends on many details of machine and compiler and needs to be determined experimentally; a value somewhere between 10 and 40 should work fine under a variety of conditions.

The pivot element is chosen by a function $pickPivotPos$ that we will not specify further. Correctness does not depend on the choice of the pivot, but efficiency does. Possible choices are: The first element, a random element, the median ("middle") element of the first three elements, or the median of a random sample of k elements for k either a small constant, say three, or a number depending on the problem size, say $\left\lceil\sqrt{r-l+1}\,\right\rceil$. The first choice requires the least amount of work, but gives little control over the size of the subproblems; the last choice requires a non-trivial but still sublinear amount of work, but yields balanced subproblems with high probability. After selecting the pivot p, we swap it into the first position of the subarray (= position ℓ of the full array).

The repeat-until loop partitions the subarray into two proper (smaller) subarrays. It maintains two indices i and j. Initially, i is at the left end of the subarray and j is at the right end;[ps was: comma] i scans to the right, and j scans to the left. After ⟸ termination of the loop we have $i=j+1$ or $i=j+2$, all elements in the subarray $a[l..j]$ are no larger than p, all elements in the subarray $a[i..r]$ are no smaller than p,

[3] Some authors propose leaving small pieces unsorted and cleaning up at the end using a single insertion sort that will be fast according to Exercise 78. Although this nice trick reduces the number of instructions executed, the solution shown is faster on modern machines because the subarray to be sorted will already be in cache.

either subarray is a proper subarray, and if $i = j+2$, $a[i+1]$ is equal to p. So we can complete the sort by recursive calls $qSort(a, \ell, j)$ and $qsort(a, i, r)$. We make these recursive calls in a non-standard fashion; this is discussed below.

Let us see in more detail how the partitioning loops work. In the first iteration of the repeat loop, i does not advance at all but stays put at ℓ, and j moves left to the rightmost element no larger than p. So j ends at ℓ or larger, generally larger. We swap $a[i]$ and $a[j]$, increment i and decrement j. In order to describe the total effect, we distinguish cases.

If p is the unique smallest element of the subarray, j moves all the way to ℓ, the swap has no effect, and $j = \ell - 1$ and $i = \ell + 1$ after the increment and decrement. We have an empty subproblem $\ell..\ell - 1$ and a subproblem $\ell + 1..r$. Partitioning is complete and both subproblems are proper subproblems.

If j moves down to $i + 1$, we swap, increment i to $\ell + 1$ and decrement j to ℓ. Partitioning is complete and we have the subproblems $\ell..\ell$ and $\ell + 1..r$. Both subarrays are proper subarrays.

If j stops at an index larger than $i + 1$, we have $\ell < i \leq j < r$ after the swap, increment of i, and decrement of j. Also, all elements left of i are at most p (and there is at least one such element) and all elements right of j are at least p (and there is at least one such element). Since the scan loop for i skips only over elements smaller than p and the scan loop for j skips only over elements larger than p, further iterations of the repeat-loop maintain this invariant. Also, all further scan loops are guaranteed to terminate by the claims in brackets and so there is no need for an index-out-bounds check in the scan loops. In other words, the scan loops are as concise as possible; they consist of a test and an increment or decrement.

Let us next study how the repeat loop terminates. If we have $i \leq j + 2$ after the scan loops, we have $i \leq j$ in the termination test. Hence, we continue the loop. If we have $i = j - 1$ after the scan loops, we swap, increment i, and decrement j. So $i = j + 1$ and the repeat-loop terminates with the proper subproblems $\ell..j$ and $i..r$. The case $i = j$ after the scan loops can only occur if $a[i] = p$. In this case the swap has no effect. After incrementing i and decrementing j we have $i = j+2$ resulting in the proper subproblems $\ell..j$ and $j+2..r$ separated by one occurence of p. We finally need to discuss the case that $i > j$ after the scan loops. Then either i goes beyond j in the first scan loop or j goes below i in the second scan loop. By our invariant, i must stop at $j+1$ in the first case and then j does not move in its scan loop or j must stop at $i-1$ in the second case. In either case we have $i = j+1$ after the scan loops. We do not swap, nor do we increment and decrement. So we have subproblems $\ell..j$ and $i..r$ and both subproblems are proper.

We have now shown that the partioning step is correct, terminates and generates proper subproblems.

Exercise 93. Is it safe to make the scan loops skip over elements equal to p? Is it safe, if it is known that the elements of the array are pairwise distinct?

Refined quicksort handles recursion in a seemingly strange way. [ps begin reformulated the old version used an not so logical order of the measures:] $\Longrightarrow$ Recall that we need to make the recursive calls $qSort(a, \ell, j)$ and $qSort(a, i, r)$. We

```
Procedure $qSort(a : Array$ of $Element;\ \ell, r : \mathbb{N})$       // Sort the subarray $a[\ell..r]$
    while $r - \ell \geq n_0$ do                                 // Use divide-and-conquer.
        $j$ :=pickPivotPos$(a, l, r)$                            // Pick a pivot element and
        swap$(a[\ell], a[j])$                                    // bring it to the first position.
        $p := a[\ell]$                                           // $p$ is the pivot now.
        $i := \ell;\ j := r$
        repeat                                                   // $a$: [$\ell$   $i\rightarrow$ $\leftarrow j$   $r$]
            while $a[i] < p$ do $i$++                            // Skip over elements
            while $a[j] > p$ do $j$--                            // already in the correct subarray.
            if $i \leq j$ then                                   // If partitioning is non yet complete,
                $swap(a[i], a[j]); i$++$; j$--                   // swap misplaced elements and go on.
        until $i > j$                                            // Partitioning is complete.
        if $i < (\ell + r)/2$ then $qSort(a, \ell, j);\ \ell := i$   // Recurse on
        else                       $qSort(a, i, r);\ r := j$     // smaller subproblem.
    endwhile
    $insertionSort(a[\ell..r])$                                  // faster for small $r - \ell$
```

Fig. 5.7. Refined quicksort

```
i →               ← j          3 6 8 1 0 7 2 4 5 9
3 6 8 1 0 7 2 4 5 9            2 0 1|8 6 7 3 4 5 9
2 6 8 1 0 7 3 4 5 9            1 0|2|5 6 7 3 4|8 9
2 0 8 1 6 7 3 4 5 9            0 1| |4 3|7 6 5|8 9
2 0 1 8 6 7 3 4 5 9               | |3 4|5 6|7|
    j i                           | |   |5 6| |
```

Fig. 5.8. Execution of $qSort$ (Figure 5.7) on $\langle 3, 6, 8, 1, 0, 7, 2, 4, 5, 9\rangle$ using the first element as the pivot and $n_0 = 1$. The left-hand side illustrates the firt partitioning step showing elements in **bold** that have just been swapped. The right-hand side shows the result of the recursive partitioning operations.

may make these calls in either order. We exploit this flexibilty by making the call for the smaller subproblem first. The call for the larger subproblem would then be the last thing done in $qSort$. This situation is known as *tail recursion* in the programming language literature. Tail recursion can be eliminted by setting the parameters (ℓ and r) to the right values and jumping to the first line of the procedure. This is precisely what the while loop does. Why is this manipulation useful? Because this guarantees that the recursion stack stays logarithmically bounded; the precise bound is $\lceil \log(n/n_0) \rceil$. This follows from the fact that we make a single recursive call for a subproblem which is at most half the size. [ps end reformulated] ⟸

Exercise 94. What is the maximal depth of the recursion stack without the "smaller subproblem first" strategy? Give a worst case example.

Exercise 95. Implement different versions of $qSort$ in your favorite programming language. Use or do not use the refinements discussed in this section and study the effect on running time and space consumption.

***Exercise 96 (Sorting Strings using Multikey Quicksort [22])** Let s be a sequence of n strings. We assume that each string ends in a special character that is different from all "normal" characters. Show that function $mkqSort(s, 1)$ below sorts a sequence s consisting of *different* strings. What goes wrong if s contains equal strings? Solve this problem. Show that the expected execution time of $mkqSort$ is $\mathcal{O}(N + n \log n)$ if $N = \sum_{e \in s} |e|$.

```
Function mkqSort(s : Sequence of String, i : ℕ) : Sequence of String
    assert $\forall e, e' \in s : e[1..i-1] = e'[1..i-1]$
    if $|s| \le 1$ then return s                                   // base case
    pick $p \in s$ uniformly at random                             // pivot character
    return concatenation of mkqSort($\langle e \in s : e[i] < p[i] \rangle$, i),
                            mkqSort($\langle e \in s : e[i] = p[i] \rangle$, i + 1), and
                            mkqSort($\langle e \in s : e[i] > p[i] \rangle$, i)
```

5.5 Selection

Selection refers to a class of problems that are easily reduced to sorting, but do not require the full power of sorting. Let $s = \langle e_1, \ldots, e_n \rangle$ be a sequence and let $s' = \langle e'_1, \ldots, e'_n \rangle$ be the sorted version of it. Selection of the smallest element requires determining e'_1, selection of the smallest and the largest requires determining e'_1 and e'_n, and selection of the k-th largest requires determining e'_k. Selection of the median refers to selecting the $\lfloor n/2 \rfloor$-th largest element. Selection of the median and also quartiles is a basic problem in statistics. It is easy to determine the smallest or the smallest and the largest element by a single scan of a sequence in linear time. We show that the k-th largest element can also be determined in linear time. The following simple recursive procedure solves the problem.

```
// Find an element with rank k
Function select(s : Sequence of Element; k : ℕ) : Element
    assert $|s| \ge k$
    pick $p \in s$ uniformly at random                       // pivot key
    a :=$\langle e \in s : e < p \rangle$
    if $|a| \ge k$ then return select(a, k)                  //
    b :=$\langle e \in s : e = p \rangle$
    if $|a| + |b| \ge k$ then return p                       //
    c :=$\langle e \in s : e > p \rangle$
    return select(c, k − |a| − |b|)                          //
```

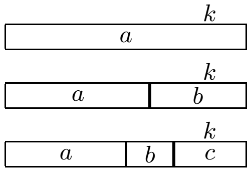


Fig. 5.9. Quickselect

The procedure is akin to quicksort and is therefore called *quickselect*. The key insight is that it suffices to follow one of the recursive calls, see Figure 5.9. As before, a pivot is chosen and the input sequence s is partitioned into subsequences a, b, and c containing the elements smaller than the pivot, equal to the pivot, and larger than the pivot, respectively. If $|a| \geq k$, we recurse on a, and if $k > |a| + |b|$, we recurse on c, of course with a suitably adjusted k. If $|a| < k \leq |a| + |b|$, the task is solved: The pivot has rank k and we return it. Observe, that the last case also covers the situation $|s| = k = 1$ and hence no special base case is needed. Figure 5.10 illustrates the execution of quickselect.

s	k	p	a	b	c
$\langle 3,1,4,5,9,\mathbf{2},6,5,3,5,8\rangle$	6	2	$\langle 1\rangle$	$\langle 2\rangle$	$\langle 3,4,5,9,6,5,3,5,8\rangle$
$\langle 3,4,5,9,\mathbf{6},5,3,5,8\rangle$	4	6	$\langle 3,4,5,5,3,4\rangle$	$\langle 6\rangle$	$\langle 9,8\rangle$
$\langle 3,4,\mathbf{5},5,3,5\rangle$	4	5	$\langle 3,4,3\rangle$	$\langle 5,5,5\rangle$	$\langle\rangle$

Fig. 5.10. The execution of $\mathit{select}(\langle 3,1,4,5,9,2,6,5,3,5,8,6\rangle, 6)$. The (**bold**) middle element of the current s is used as the pivot p.

As for quicksort, the worst case execution time of quickselect is quadratic. But the expected execution time is linear and hence a logarithmic factor faster than quicksort.

Theorem 19. *Algorithm quickselect runs in expected time $\mathcal{O}(n)$ on an input of size n.*

Proof. We will give an analysis that is simple and shows linear expectation. It does not give the smallest constant possible. Let $T(n)$ denote the expected execution time of quickselect. Call a pivot *good* if neither $|a|$ nor $|b|$ are larger than $2n/3$. Let γ denote the probability that the pivot is good. Then $\gamma \geq 1/3$. We now make the conservative assumption that the problem size in the recursive call is only reduced for good pivots and that even then it is only reduced by a factor of $2/3$. Since the work outside the recursive call is linear in n, there is an appropriate constant c such that

$$\begin{aligned} T(n) &\leq cn + \gamma T\left(\frac{2n}{3}\right) + (1-\gamma)T(n) \qquad \text{or, equivalently} \\ T(n) &\leq \frac{cn}{\gamma} + T\left(\frac{2n}{3}\right) \leq 3cn + T\left(\frac{2n}{3}\right) \leq 3c\left(n + \frac{2n}{3} + \frac{4n}{9} + \ldots\right) \\ &\leq 3cn \sum_{i \geq 0} \left(\frac{2}{3}\right)^i \leq 3cn \frac{1}{1-2/3} = 9cn\ . \end{aligned}$$

Exercise 97. Modify quickselect so that it returns the k smallest elements.

Exercise 98. Give a selection algorithm that permutes an array in such a way that the k smallest elements are in entries $a[1], \ldots, a[k]$. No further ordering is required except that $a[k]$ should have rank k. Adapt the implementation tricks from array-based quicksort to obtain a nonrecursive algorithm with fast inner loops.

Exercise 99 (Streaming selection).

1. Develop an algorithm that finds the k-th smallest element of a sequence that is presented to you one element at a time in an order you cannot control. You have only space $\mathcal{O}(k)$ available. This models a situation where voluminous data arrives over a network or at a sensor.
2. Refine your algorithm so that it achieves running time $\mathcal{O}(n \log k)$. You may want to read some of Chapter 6 first.

*c) Refine the algorithm and its analysis further so that your algorithm runs in average case time $\mathcal{O}(n)$ if $k = \mathcal{O}(n/\log n)$. Here, average means that all presentation orders of elements in the sequence are equally likely.

5.6 Breaking the Lower Bound

The title of this section is, of course, non-sense. A lower bound is an absolute statement. It states that in a certain model of computation a certain task cannot be carried out faster than the bound. So a lower bound cannot be broken. Be careful. It cannot be broken within the model of computation. It does not exclude the possibility that a faster solution exists in a richer model of computation. In fact, we may even interpret the lower bound as a guideline for getting faster. It tells us that we must enlarge our repertoire of basic operations in order to get faster.

What does this mean for sorting? So far, we restricted ourselves to comparison-based sorting. The only way to learn about the order of items was by comparing two of them. For structured keys, there are more effective ways to gain information and this will allow us to break the $\Omega(n \log n)$ lower bound valid for comparison-based sorting. For example, numbers and strings have structure; they are sequences of digits and characters, respectively.

Let us start with a very simple algorithm *Ksort* that is fast if the keys are small integers, say in the range $0..K-1$. The algorithm runs in time $\mathcal{O}(n+K)$. We use an array $b[0..K-1]$ of *buckets* that are initially empty. Then we scan the input and insert an element with key k into bucket $b[k]$. This can be done in constant time per element, for example, by using linked lists for the buckets. Finally, we append all the nonempty buckets to obtain a sorted output. Figure 5.11 gives the pseudocode. For example, if elements are pairs whose first element is a key in range $0..3$ and

$$s = \langle (3,a),(1,b),(2,c),(3,d),(0,e),(0,f),(3,g),(2,h),(1,i)\rangle$$

we obtain $b = [\langle (0,e),(0,f)\rangle,\ \langle (1,b),(1,i)\rangle,\ \langle (2,c),(2,h)\rangle,\ \langle (3,a),(3,d),(3,g)\rangle]$ and output $\langle (0,e),(0,f),(1,b),(1,i),(2,c),(2,h),(3,a),(3,d),(3,g)\rangle$. The example illustrates an important property of $Ksort$. It is *stable*, i.e., elements with the same key inherit their relative order from the input sequence. Here it is crucial that elements are *appended* to their respective bucket.

$KSort$ can be used as a building block for sorting larger keys. The idea behind *radix sort* is to view integer keys as numbers represented by digits in the range

```
Procedure KSort(s : Sequence of Element)
    b = ⟨⟨⟩, ..., ⟨⟩⟩ : Array [0..K − 1] of Sequence of Element
    foreach $e \in s$ do $b[key(e)].pushBack(e)$          //
    $s :=$ concatenation of $b[0], \ldots, b[K-1]$
```

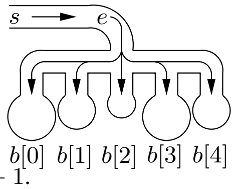


Fig. 5.11. Sorting with keys in the range $0..K-1$.

```
Procedure LSDRadixSort(s : Sequence of Element)
    for $i := 0$ to $d - 1$ do
        redefine $key(x)$ as $(x \operatorname{div} K^i) \bmod K$          // x
        KSort(s)
        invariant s is sorted with respect to digits $i..0$
```

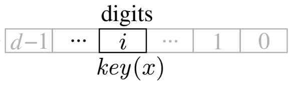


Fig. 5.12. Sorting with keys in the range $0..K^d - 1$ using **L**east **S**ignificant **D**igit radix sort.

```
Procedure uniformSort(s : Sequence of Element)
    $n := |s|$
    b = ⟨⟨⟩, ..., ⟨⟩⟩ : Array [0..n − 1] of Sequence of Element
    foreach $e \in s$ do $b[\lfloor key(e) \cdot n \rfloor].pushBack(e)$
    for $i := 0$ to $n - 1$ do sort $b[i]$ in time $\mathcal{O}(|b[i]| \log |b[i]|)$
    $s :=$ concatenation of $b[0], \ldots, b[n-1]$
```

Fig. 5.13. Sorting random keys in the range $[0, 1)$.

$0..K-1$. Then $KSort$ is applied once for each digit. Figure 5.12 gives a radix-sorting algorithm for keys in the range $0..K^d - 1$ that runs in time $\mathcal{O}(d(n+K))$. The elements are sorted first by their least significant digit then by the second least significant digit and so on until the most significant digit is used for sorting. It is not obvious why this works. Correctness rests on the stability of $Ksort$. Since $KSort$ is stable, the elements with the same i-th digit remain sorted with respect to digits $i-1..0$ during the sorting process with respect to digit i. For example, if $K = 10$, $d = 3$, and

$$s = \langle 017, 042, 666, 007, 111, 911, 999 \rangle, \text{ we successively obtain}$$
$$s = \langle 11\mathbf{1}, 91\mathbf{1}, 04\mathbf{2}, 66\mathbf{6}, 01\mathbf{7}, 00\mathbf{7}, 99\mathbf{9} \rangle,$$
$$s = \langle 0\mathbf{07}, 1\mathbf{11}, 9\mathbf{11}, 0\mathbf{17}, 0\mathbf{42}, 6\mathbf{66}, 9\mathbf{99} \rangle, \text{ and}$$
$$s = \langle \mathbf{007}, \mathbf{017}, \mathbf{042}, \mathbf{111}, \mathbf{666}, \mathbf{911}, \mathbf{999} \rangle \ .$$

The mechanical sorting machine shown on Page 99 basically implemented one pass of radix sort and was most likely used to run LSD radix sort.

Radix sort starting with the most significant digit (*MSD radix sort*) is also possible. We apply $KSort$ to the most significant digit and then sort each bucket recursively. The only problem is that the buckets might be much smaller than K so that it would be expensive to apply $KSort$ to small buckets. We then have to switch to another algorithm. This works particularly well if we can assume that the keys are uniformly distributed. More specifically, let us now assume that keys are real numbers with $0 \leq \mathit{key}(e) < 1$. Algorithm *uniformSort* from Figure 5.13 scales these keys to integers between 0 and $n-1 = |s|-1$, and groups them into n buckets where bucket $b[i]$ is responsible for keys in the range $[i/n, (i+1)/n)$. For example, if $s = \langle 0.8, 0.4, 0.7, 0.6, 0.3\rangle$ we obtain five buckets responsible for intervals of size 0.2 and

$$b = [\langle\rangle, \quad \langle 0.3\rangle, \quad \langle 0.4\rangle, \quad \langle 0.6, 0.7\rangle, \quad \langle 0.8\rangle]$$

and only $b[3] = \langle 0.7, 0.6\rangle$ is a non-trivial subproblem. *uniformSort* is very efficient for *random* keys.

Theorem 20. *If keys are independent uniformly distributed random values in* $[0.1)$, *uniformSort sorts* n *keys in expected time* $\mathcal{O}(n)$ *and worst case time* $\mathcal{O}(n \log n)$.

Proof. We leave the worst case bound as an exercise and concentrate on the average case. Total execution time T is $\mathcal{O}(n)$ for setting up the buckets and concatenating the sorted buckets plus the time for sorting the buckets. Let T_i denote the time for sorting the i-th bucket. We obtain

$$\mathrm{E}[T] = \mathcal{O}(n) + \mathrm{E}[\sum_{i<n} T_i] = \mathcal{O}(n) + \sum_{i<n} \mathrm{E}[T_i] = n\mathrm{E}[T_0] \ .$$

The first equality follows from linearity of expectation (Equation (A.2)) and the second equality uses that all bucket sizes have the same distribution for uniformly distributed inputs. Hence, it remains to show that $\mathrm{E}[T_0] = \mathcal{O}(1)$. We prove the stronger claim that $\mathrm{E}[T_0] = \mathcal{O}(1)$ even if a quadratic time algorithm such as insertion sort is used for sorting the buckets. The analysis is similar to the arguments used to analyse the behavior of hashing in Chapter 4.

Let $B_0 = |b[0]|$. We have $\mathrm{E}[T_0] = \mathcal{O}\big(\mathrm{E}[B_0^2]\big)$. The random variable B_0 obeys a binomial distribution (Equation (A.7)) with n trials and success probability $1/n$ and hence

$$\mathrm{prob}(B_0 = i) = \binom{n}{i}\frac{1}{n^i}\left(1 - \frac{1}{n}\right)^{n-i} \leq \frac{n^i}{i!}\frac{1}{n^i} \leq \frac{1}{i!} \leq \left(\frac{e}{i}\right)^i \ ,$$

where the last inequality follows from Stirling's approximation of the factorial (Equation (A.9)). We obtain

$$\begin{aligned}
\mathrm{E}[B_0^2] &= \sum_{i \leq n} i^2 \mathrm{prob}(B_0 = i) \leq \sum_{i \leq n} i^2 \left(\frac{e}{i}\right)^i \\
&\leq \sum_{i \leq 5} i^2 \left(\frac{e}{i}\right)^i + e^2 \sum_{i \geq 6} \left(\frac{e}{i}\right)^{i-2} \\
&\leq \mathcal{O}(1) + e^2 \sum_{i \geq 6} \left(\frac{1}{2}\right)^{i-2} = \mathcal{O}(1)
\end{aligned}$$

and hence $\mathrm{E}[T] = \mathcal{O}(n)$.

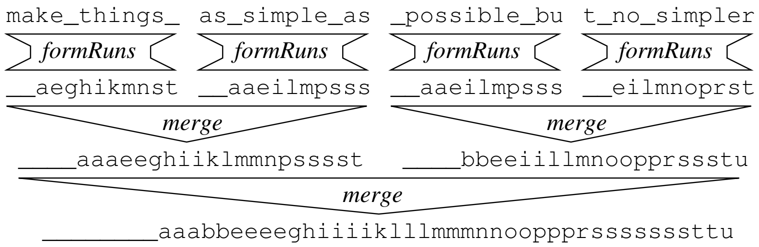


Fig. 5.14. An example of two-way mergesort with initial runs of length 12.

***Exercise 100** Implement an efficient sorting algorithm for elements with keys in the range $0..K-1$ that uses the data structure from Exercise 47 as input and output. Space consumption should be $n + \mathcal{O}(n/B + KB)$ for n elements and blocks of size B.

5.7 External Sorting

Sometimes data is so huge that it does not fit into internal memory. In this section we will learn how to sort such data sets in the external memory model introduced in Section 2.2. It distinguishes between a fast internal memory of size M and a large external memory. Data is moved in the memory hierarchy in blocks of size B. Scanning data is fast in external memory and mergesort is based on scanning. We therefore take mergesort as the starting point for external memory sorting.

Assume the input is given as an array in external memory. We describe a nonrecursive implementation for the case that the number of elements n is divisible by B. We load subarrays of size M into internal memory, sort them using our favorite algorithm, e.g., *qSort*, and write the sorted subarrays back to external memory. We refer to the sorted subarrays as *runs*. The *run formation phase* takes n/B block reads and n/B block writes, i.e., a total of $2n/B$ I/Os. Then we merge pairs of runs into larger runs in $\lceil \log(n/M) \rceil$ *merge phases* ending up with a single sorted run. Figure 5.14 gives an example for $n = 48$ and runs of length twelve.

How do we merge two runs? We keep one block from each of the two input runs and the output run in internal memory. We call these blocks *buffers*. Initially, the input buffers are filled with the first B elements of the input runs and the output buffer is empty. We compare the leading elements of the input buffers and move the smaller one to the output buffer. If an input buffer becomes empty, we fetch the next block of the corresponding input run, if the output buffer is full, we write it to external memory.

Each merge phase reads all current runs and writes new runs of twice the length. Therefore each phase needs n/B block reads and n/B block writes. Summing over all phases, we obtain $2n/B(1 + \lceil \log n/M \rceil)$ I/Os. The technique works provided that $M \geq 3B$.

Multiway Mergesort

In general, internal memory can hold many blocks and not just three. We will describe how to make full use of the available internal memory during merging. The idea is to merge more than just two runs; this will reduce the number of phases. In *k-way merging*, we merge k sorted sequences into a single output sequence. In each step we find the input sequence with the smallest first element. This element is removed and appended to the output sequence. External memory implementation is easy as long as we have enough internal memory for k input buffer blocks, one output buffer block, and a small amount of additional storage.

For each sequence, we need to remember which element we are currently considering. To find the smallest element among all k sequences, we keep their current elements in a *priority queue*. A priority queue maintains a set of elements supporting the operations insertion and deletion of the minimum. Chapter 6 explains how priority queues can be implemented so that insertion and deletion take time $\mathcal{O}(\log k)$ for k elements. The priority queue tells us in each step which sequence contains the smallest element. We delete it from the priority queue, move it to the output buffer, and insert the next element from the corresponding input buffer into the priority queue. If an input buffer runs dry, we fetch the next block of the corresponding sequence and if the output buffer becomes full, we write it to the external memory.

How large can we choose k? We need to keep $k + 1$ blocks in internal memory and we need a priority queue for k keys. So we need $(k + 1)B + O(k) \leq M$ or $k = O(M/B)$. The number of merging phases is reduced to $\lceil \log_k(n/M) \rceil$ and hence the total number of I/Os becomes

$$2\frac{n}{B}\left(1 + \left\lceil \log_{M/B} \frac{n}{M} \right\rceil\right) . \tag{5.1}$$

The difference to binary merging is the much larger base of the logarithm. Interestingly, the above upper bound for the I/O-complexity of sorting is also a lower bound [4], i.e., under fairly general assumptions, no external sorting algorithm with less I/O operations is possible.

In practice, the number of merge phases will be very small. Observe that a single merge phase suffices as long as $n \leq M^2/B$. We first form M/B runs of length M each and then merge these runs into a single sorted sequence. If internal memory stands for DRAMs and external memory stands for disks, this bound on n is no real restriction for all practical system configurations.

Exercise 101. Show that multiway mergesort needs only $\mathcal{O}(n \log n)$ element comparisons.

Exercise 102 (Balanced systems). Study the current market prices of computers, internal memory, and mass storage (currently hard disks). Also estimate the block size needed to achieve good bandwidth for I/O. Can you find any configuration where multi-way mergesort would require more than one merging phase for sorting an input filling all the disks in the system? If so, which fraction of the system cost would you have to spend on additional internal memory to go back to a single merging phase?

Sample Sort

The most popular internal memory sorting algorithm is not mergesort but quicksort. So it is natural to look for an external memory sorting algorithm based on quicksort. We will sketch *Sample sort*. It has the same performance guarantee as multiway mergesort (Expression 5.1), however only in expectation and not worst case. It is is easier to adapt to parallel disks and parallel processors than merging-based algorithms. Furthermore, similar algorithms can be used for fast external sorting of integer keys along the lines of Section 5.6.

Instead of the single pivot element of quicksort, we now use $k-1$ *splitter elements* $s_1,\ldots,\ s_{k-1}$ to split an input sequence into k output sequences or *buckets*. Bucket i gets the elements e with $s_{i-1} \leq e < s_i$. To simplify matters we define the artificial splitters $s_0 = -\infty$ and $s_k = \infty$ and we assume that all elements have different keys. The splitters should be chosen in such a way that the buckets have a size of roughly n/k. The buckets are then sorted recursively. In particular, buckets that fit into the internal memory can subsequently be sorted internally. Note the similarity to MSB-radix sort in Section 5.6.

The main challenge is to find good splitters quickly. Sample sort uses a fast and simple randomized strategy. For some integer a, we randomly choose $ak+k-1$ *sample* elements from the input. The sample S is then sorted internally and we define the splitters as $s_i = S[(a+1)i]$ for $1 \leq i \leq k-1$, i.e., subsequent splitters are separated by a samples, the first splitter is preceded by a samples, and the last splitter is followed by a samples. Taking $a=0$ results in a small sample set, but splitting will not be very good. Moving all elements to the sample will result in perfect splitters, but the sample is too big. The analysis shows that setting $a = \mathcal{O}(\log k)$ achieves roughly equal bucket sizes at low cost for sampling and sorting the sample.

The most I/O-intensive part of sample sort is k-way distribution of the input sequence to the buckets. We keep one buffer block for the input sequence and one buffer block for each bucket. These buffers are handled analogously to the buffer blocks in k-way merging. If the splitters are kept in a sorted array, we can find the right bucket for an input element e in time $\mathcal{O}(\log k)$ using binary search.

Theorem 21. *Sample sort sorts n inputs using*

$$\mathcal{O}\Big(\frac{n}{B}\left(1+\left\lceil\log_{M/B}\frac{n}{M}\right\rceil\right)\Big)$$

expected I/O steps. Internal work is $\mathcal{O}(n\log n)$.

We leave the detailed proof to the reader and explain only the key ingredient of the analysis. We use $k = \Theta(\min(n/M, M/B))$ buckets and a sample of size $\mathcal{O}(k\log k)$. The following lemma shows that with this sample size, it is unlikely that any bucket has size much larger than average. We hide the constant factors behind $\mathcal{O}(\cdot)$-notation because our analysis is not very tight in this respect.

Lemma 16. *Let $k \geq 2$ and $a+1 = 12\ln k$. A sample of size $(a+1)k-1$ suffices to ensure that no bucket receives more than $4n/k$ elements with probability at least $1/2$.*

Proof. As in our analysis of quicksort (Theorem 18), it is useful to study the sorted version $s' = \langle e'_1, \ldots, e'_n \rangle$ of the input. Assume there is a bucket with at least $4n/k$ elements assigned to it. We estimate the probability of this event.

We split s' into $k/2$ segments of length $2n/k$. The j-th segment t_j contains elements $e'_{2jn/k+1}$ to $e'_{2(j+1)n/k}$. If $4n/k$ elements end up in some bucket there must be some segment t_j such that all its elements end up in the same bucket. This can only happen if less than $a+1$ samples are taken from t_j because otherwise at least one splitter would be chosen from t_j and its elements would not end up in a single bucket. Let us concentrate on a fixed j.

We use random variable X to denote the number of samples taken from t_j. Recall that we take $(a+1)k-1$ samples. For each sample i, $1 \leq i \leq (a+1)k-1$, we define an indicator variable X_i with $X_i = 1$ if the i-th sample is taken from t_j and $X_i = 0$ otherwise. Then $X = \sum_{1 \leq i \leq (a+1)k-1} X_i$. Also, the X_i's are independent and $\operatorname{prob}(X_i = 1) = 2/k$. Independence allows us to use the so-called Chernoff bound (A.5) to estimate the probability that $X < a+1$. We have $\mathrm{E}[X] = ((a+1)k - 1) \cdot \frac{2}{k} = 2(a+1) - 2/k \geq 3(a+1)/2$. Hence $X < a+1$ implies $X < (1-1/3)\mathrm{E}[X]$ and so we can use (A.5) with $\epsilon = 1/3$. Thus

$$\operatorname{prob}(X < a+1) \leq e^{-(1/9)\mathrm{E}[X]/2} \leq e^{-(a+1)/12} = e^{-\ln k} = \frac{1}{k} \,.$$

The probability that an insufficient number of samples is chosen from a fixed t_j is thus at most $1/k$ and hence the probability that an insufficient number is chosen from some t_j is at most $(k/2) \cdot (1/k) = 1/2$. Thus with probability at least $1/2$, each bucket receives less than $4n/k$ elements.

Exercise 103. Work out the details of an external memory implementation of Sample sort. In particular, explain how to implement multi-way distribution using $2n/B + k + 1$ I/O steps if the internal memory is large enough to store $k+1$ blocks of data and $\mathcal{O}(k)$ additional elements.

Exercise 104 (Many equal keys). Explain how to generalize multiway distribution so that it still works if some keys occur very often. Hint: there are at least two different solutions. One uses the sample to find out which elements are frequent. Another solution makes all elements unique by interpreting an element e at input position i as the pair (e, i).

***Exercise 105 (More accurate distribution.)** A sample of size $\mathcal{O}\big((k/\epsilon^2)\log(k/\epsilon m)\big)$ guarantees with probability at least $1 - 1/m$ that no bucket has more than $(1+\epsilon)n/k$ elements. (Can you even get rid of the ϵ in the logarithmic factor?)

5.8 Implementation Notes

Comparison-based sorting algorithms are usually available in standard libraries so that you may not have to implement one yourself. Many libraries use tuned implementations of quicksort.

```
Procedure KSortArray(a,b : Array [1..n] of Element)
    c = ⟨0, ..., 0⟩ : Array [0..K − 1] of ℕ        // counters for each bucket
    for i := 1 to n do  c[key(a[i])]++             // Count bucket sizes
    C := 0
    for k := 0 to K − 1 do  (C, c[k]) := (C + c[k], C)   // Store $\sum_{i<k} c[k]$ in c[k].
    for i := 1 to n do                             // Distribute a[i]
        b[c[key(a[i])]] := a[i]
        c[key(a[i])]++
```

Fig. 5.15. Array-based sorting with keys in the range $0..K-1$. The input is an unsorted array a. The output is b with the elements of a in sorted order. We first count the number of inputs for each key. Then we form the partial sums of the counts. Finally, we write each input element to the correct position in the output array.

Canned non-comparison based-sorting routines are less readily available. Figure 5.15 shows a careful array-based implementation of Ksort. It works well for small to medium-sized problems. For large inputs, it suffers from the problem that the distribution of elements to buckets causes a cache fault for every element.

To fix this problem one can use multi-phase algorithms similar to MSD-radix sort. The number K of output sequences should be chosen in such a way that one block from each bucket is kept in the cache[4]. The distribution degree K can be larger when the subarray to be sorted fits into the cache. We can then switch to a variant of Algorithm *uniformSort* in Figure 5.13.

Another important practical aspect concerns the type of elements to be sorted. Sometimes, we have rather large elements that are sorted with respect to small keys. For example, you may want to sort an employee database by last name. In this situation, it makes sense to first extract the keys and store them in an array together with pointers to the original elements. Then only the key-pointer pairs are sorted. If the orginal elements need to be brought into sorted order, they can be permuted accordingly in linear time using the sorted key-pointer pairs.

Multiway merging of a small number of sequences (perhaps up to eight) deserves special mentioning. In this case, the tournament tree can be kept in the processor registers [150, 193].

C/C++:

Sorting is one of the few algorithms that is part of the C standard library. However, the C-sorting routine *qsort* is slower and harder to use than the C++–function *sort*. The main reason is that the comparison function is passed as a function pointer and is then called for every element comparison. In contrast, *sort* uses the template mechanism of C++ to figure out at compile time how comparisons are performed so that

[4] If there are M/B cache blocks this does *not* mean that we can use $k = M/B - 1$. A discussion of this issue can be found in [129].

the code generated for comparisons is often a single machine instruction. The parameters passed to $sort$ are an iterator pointing to the start of the sequence to be sorted and an iterator pointing after the end of the sequence. Hence, sort can be applied to lists, arrays, etc. In our experiments on an Intel Pentium III and gcc 2.95, sort on arrays runs faster than our manual implementation of quicksort. One possible reason is that compiler designers may tune there code optimizers until they find that good code for the library version of quicksort is generated. There is an efficient parallel disk external memory sorter in the STXXL [50], an external memory implementation of the STL. Efficient parallel sorters (parallel quicksort and parallel multiway mergesort) for multicore machines are available with the Multi-Core STL [**?**][todo
$\Longrightarrow$ url][part of gcc?].
$\Longrightarrow$

Java:

The Java 6 platform provides a method $sort$ which implements stable binary mergesort for $Arrays$ and $Collections$. One can use a customizable $Comparator$ but there is also a default implementation for all classes supporting the interface $Comparable$.

$\Longrightarrow$ [C# ??? check everywhere]

Exercise 106. Give a C or C++-implementation of the quicksort in Figure 5.7 that uses only two parameters: A pointer to the (sub)array to be sorted, and its size.

5.9 Historical Notes and Further Findings

In later chapters we will discuss several generalizations of sorting. Chapter 6 discusses priority queues, a data structure supporting insertions and removal of the smallest element. In particular, inserting n elements followed by repeated deletion of the minimum amounts to sorting. Fast priority queues result in quite good sorting algorithms. A further generalization are the *search trees* introduced in Section 7, a data structure for maintaining a sorted list that allows searching, inserting, and removing elements in logarithmic time.

We have seen several simple, elegant, and efficient randomized algorithms in this chapter. An interesting question is whether these algorithms can be replaced by deterministic ones. Blum et al. [26] describe a deterministic median selection algorithm that is similar to the randomized algorithm from Section 5.5. This algorithm makes pivot selection more reliable using recursion: It splits the input set into subsets of five elements, determines the median of each subset by sorting the five-element subset, then determines the median of the $n/5$ medians by calling the algorithm recursively, and finally uses the median of the medians as the splitter. The resulting algorithm has linear worst case execution time (we invite the reader to set up a recurrence for the running time and to show that it has a linear solution), but the large constant factor makes the algorithm impractical.

There are quite practical ways to reduce the expected number of comparisons required by quicksort. Using the median of three random elements yields an algorithm with about $1.188n \log n$ comparisons. The median of three medians of three-element subsets brings this down to $\approx 1.094n \log n$ [20]. The number of comparisons can be reduced further by making the number of elements considered for pivot selection dependent on the size of the subproblem. Martinez and Roura [119] show that for a subproblem of size m, the median of $\Theta(\sqrt{m})$ elements is a good choice for the pivot. With this approach, the total number of comparisons becomes $(1 + o(1))n \log n$, i.e., matches the lower bound of $n \log n - \mathcal{O}(n)$ up to lower order terms. Interestingly, the above optimizations can be counterproductive. Although less instructions are executed, it becomes impossible to predict when the inner while-loops of quicksort are aborted. Since modern, deeply pipelined processors only work efficiently when they can predict the directions of branches taken, the net effect on performance can even be negative [**?**]. Therefore, [157] develops a comparison based sorting algorithm that avoids conditional branch instructions. An interesting deterministic variant of quicksort is proportion-extend sort [39].

A classical sorting algorithm of some historical interest is *Shell sort* [98, 163], a generalization of insertion sort, that gains efficiency by also comparing nonadjacent elements. It is still open whether some variant of Shellsort achieves $\mathcal{O}(n \log n)$ average running time [98, 120].

There are some interesting techniques for improving external multiway mergesort. The *snow plow* heuristic [109, Section 5.4.1] forms runs of expected size $2M$ using a fast memory of size M: Whenever an element is selected from the internal priority queue and written to the output buffer and the next element in the input buffer can extend the current run, we add it to the priority queue. Also, the use of *tournament trees* instead of general priority queues leads to a further improvement of multiway merging [109].

Parallelism can be used to improve sorting very large data sets, either in the form of a uni-processor using parallel disks or in the form of a multi-processor. Multiway mergesort and distribution sort can be adapted to D parallel disks by *striping*, i.e., any D consecutive blocks in a run or bucket are evenly distributed over the disks. Using randomization, this idea can be developed into almost optimal algorithms that also overlaps I/O and computation [51]. The sample sort algorithm of Section 5.7 can be adapted to parallel machines [25] and results in an efficient parallel sorter.

We have seen linear time algorithms for highly structured inputs. A quite general model, for which the $n \log n$ lower bound does not hold, is the *word model*. In this model, keys are integers that fit into a single memory cell, say 32 or 64 bit keys, and the standard operations on words (bitwise-and, bitwise-or, addition, ...) are available in constant time. In this model, sorting is possible in deterministic time $\mathcal{O}(n \log \log n)$ [9]. With randomization even $\mathcal{O}\left(n\sqrt{\log \log n}\right)$ is possible [196]. *Flash sort* [141] is a distribution-based algorithm that works almost in-place.

Exercise 107 (Unix spell checking). Assume you have a dictionary consisting of a sorted sequence of correctly spelled words. To check a text, convert it to a sequence of words, sort it, scan text and dictionary simultaneously, and output the words in the text that do not appear in the dictionary. Implement this spell checker using unix tools in a small number of lines of code. Can you do it in one line?

6

Priority Queues

Company TMG markets tailor-made first-rate garments. It organizes marketing, measurements etc., but outsources the actual fabrication to independent tailors. The company keeps 20% of the revenue. When the company was founded in the 19th century, there were five subcontractors. Now it controls 15 % of the world market and there are thousands of subcontractors worldwide.

Your task is to assign orders to the subcontractors. The rule is that an order is assigned to the tailor who has so far (in the current year) been assigned the smallest total value of orders. Your ancestors used a blackboard to keep track of the current sum of orders for each tailor; in computer science terms, they kept a list of values and spent linear time to find the correct tailor. The business has outgrown this solution. Can you come up with a more scalable solution where you have to look only at a small number of values to decide who will be assigned the next order?

In the following year the rules are changed. In order to encourage timely delivery, the orders are now assigned to the tailor with the smallest value of unfinished *orders, i.e, whenever a finished order arrives, you have to deduct the value of the order from the backlog of the tailor who executed it. Is your strategy for assigning orders flexible enough to handle this efficiently?*

Priority Queues are the data structure required for the problem above and for many other applications. We start our discussion with the precise specification. Priority queues maintain a set M of $\mathit{Element}$s with Keys under the following operations:

$M.\mathit{build}(\{e_1,\ldots,e_n\})$: $M := \{e_1,\ldots,e_n\}$
$M.\mathit{insert}(e)$: $M := M \cup \{e\}$
$M.\min$: **return** $\min M$
$M.\mathit{deleteMin}$: $e := \min M$; $M := M \setminus \{e\}$; **return** e

This is enough for the first part of our example: Each year we build a new priority queue containing an $\mathit{Element}$ with Key zero for each contract tailor. To assign an order, we delete the smallest $\mathit{Element}$, add the order value to its Key, and reinsert it. Section 6.1 presents a simple and efficient implementation of this basic functionality.

Addressable priority queues additionally support operations on arbitrary elements addressed by an element handle h.

insert: As before but return a handle to the element inserted.
$\mathit{remove}(h)$: Remove the element specified by handle h.

$decreaseKey(h, k)$: Decrease the key of the element specified by handle h to k.
$Q.merge(Q')$: $Q := Q \cup Q'$; $Q := \emptyset$.

In our example, operation $remove$ might be helpful when a contractor is fired because it delivers poor quality. Together with $insert$ we can also implement the "new contract rules": When an order is delivered, we remove the $Element$ for the contractor who executed the order, subtract the value of the order from its Key value, and reinsert the $Element$. $DecreaseKey$ streamlines this process to a single operation. In Section 6.2 we will see that this is not just convenient but that decreasing keys can be implemented more efficiently than arbitrary element updates.

Priority queues have many applications. [VorwÃď'rtsverweis auf machine $\Longrightarrow$ scheduling wieder reinbauen.] For example, the rather naive selection-sort algorithm from Section 5.1 can be implemented efficiently now: First insert all elements into a priority queue. Then repeatedly delete the smallest element and output it. A tuned version of this idea is described in Section 6.1. The resulting *heapsort* algorithm is popular because it needs no additional space and is worst-case efficient.

In a *discrete event simulation* one has to maintain a set of pending events. Each event happens at some scheduled point in time and creates zero or more new events in the future. Pending events are kept in a priority queue. The main loop of the simulation deletes the next event from the queue, executes it, and inserts newly generated events into the priority queue. Note that priorities (times) of the deleted elements (simulated events) are monotonically increasing during the simulation. It turns out that many applications of priority queues have this monotonicity property. Section 10.4 explains how to exploit monotonicity for integer keys.

Another application of monotone priority queues is the *best first branch-and-bound* approach to optimization described in Section 12.4. Here elements are partial solutions of an optimization problem and the keys are optimistic estimates of the obtainable solution quality. The algorithm repeatedly removes the best looking partial solution, refines it, and inserts zero or more new partial solutions.

We will see two applications of addressable priority queues in the chapters on graph algorithms. In both applications the priority queue stores nodes of a graph. Dijkstra's algorithm for computing shortest paths (Section 10.3) uses a monotone priority queue where the keys are path lengths. The Jarník-Prim algorithm for computing minimum spanning trees (Section 11.2) uses a (non-monotone) priority queue where the keys are the weights of edges connecting a node to a partial spanning tree. In both algorithms, there can be a $decreaseKey$ operation for each edge whereas there is at most one $insert$ and $deleteMin$ for each node. Observe that the number of edges may be much larger than the number of nodes and hence the implemention of $decreaseKey$ deserves special attention.

Exercise 108. Show how to implement bounded non-addressable priority queues by arrays. The maximal size of the queue is w and when the queue has size n, the first n entries of the array are used. Compare the complexity of the queue operations for two naive implementations. In the first implementation the array is unsorted and in the second implementation the array is sorted.

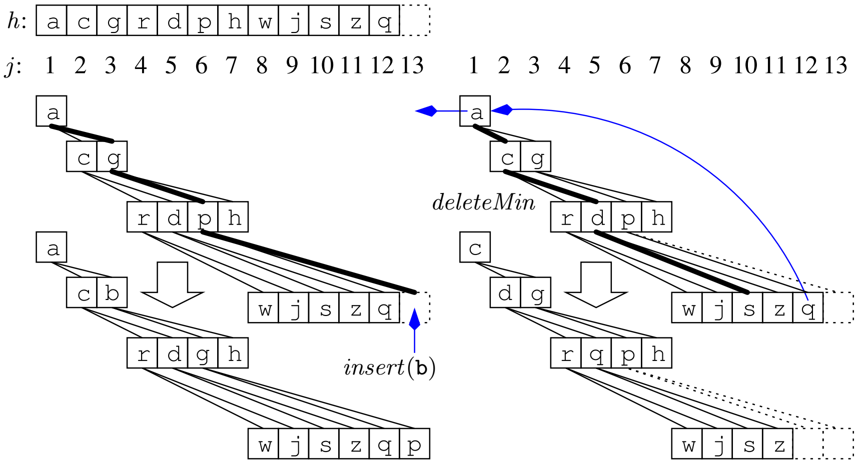


Fig. 6.1. The top part shows a heap with $n = 12$ elements stored in an array h with $w = 13$ entries. The root has number one. The children of the root have numbers 2 and 3. The children of node i have numbers $2i$ and $2i+1$ (if they exist). The parent of a node i, $i \geq 2$, has number $\lfloor i/2 \rfloor$. The elements stored in this implicitly defined tree fulfill the invariant that parents are no larger than their children, i.e., the tree is heap-ordered. The left part shows the effect of inserting b. The fat edges mark a path from the rightmost leaf to the root. The new element b is moved up this path until its parent is smaller. The remaining elements on the path are moved down to make room for b. The right part shows the effect of deleting the minimum. The fat edges mark the path p starting at the root and always proceeding to the child with smaller *Key*. *Element* q is provisionally moved to the root and then moves down path p until its successors are larger. The remaining elements move up to make room for q.

Exercise 109. Show how to implement addressable priority queues by doubly linked lists. Each list item represents an element in the queue and a handle is a handle of a list item. Compare the complexity of the queue operations for two naive implementations. In the first implementation the list is unsorted and in the second implementation the list is sorted.

6.1 Binary Heaps

Heaps are a simple and efficient implementation of non-addressable bounded priority queues. They can be made unbounded in the same way as bounded arrays are made unbounded in Section 3.2. Heaps can also be made addressable, but we will see better addressable queues in later sections.

We use an array $h[1..w]$ that stores the elements of the queue. The first n entries of the array are used. The array is *heap-ordered*, i.e.,

$$\text{if } 2 \leq j \leq n \text{ then } h[\lfloor j/2 \rfloor] \leq h[j]\,.$$

```
Class BinaryHeapPQ($w : \mathbb{N}$) of Element
    $h : Array\ [1..w]$ of Element                          // The heap $h$ is
    $n = 0 : \mathbb{N}$                                     // initially empty and has the
    invariant $\forall j \in 2..n : h[\lfloor j/2 \rfloor] \leq h[j]$      // heap property which implies that
    Function min assert $n > 0$ ; return $h[1]$              // the root is the minimum.
```

Fig. 6.2. Class declaration for a priority queue based on binary heaps whose size is bounded by w.

What does this mean? The key to understanding this definition is a bijection between positive integers and the nodes of a complete binary tree as illustrated in Figure 6.1. In a heap the minimum element is stored in the root (= array position 1). Thus $\min$ takes time $\mathcal{O}(1)$. Creating an empty heap with space for w elements also takes constant time as it only needs to allocate an array of size w. Figure 6.2 gives pseudocode for this basic setup.

The minimum of a heap is stored in $h[1]$ and hence can be found in constant time; this is the same as for a sorted array. However, the heap property is much less restrictive than the property of being sorted. For example, there is only one sorted version of the set $\{1,2,3\}$, but both $\langle 1,2,3 \rangle$ and $\langle 1,3,2 \rangle$ are legal heap representations.

Exercise 110. Give all representations of $\{1,2,3,4\}$ as a heap.

We will next see that the increased flexibility permits efficient implementations of $insert$ and $deleteMin$. We choose a description which is simple and can be easily proven correct. Section 6.4 gives some hints towards a more efficient implementation. An $insert$ puts a new element e tentatively at the end of the heap h, i.e., into $h[n]$ and then moves e to an appropriate position on the path from leaf $h[n]$ to the root.

```
Procedure insert($e : Element$)
    assert $n < w$
    $n$++; $h[n] := e$
    $siftUp(n)$
```

where $siftUp(s)$ moves the contents of node s towards the root until the heap property holds, cf. Figure 6.1.

```
Procedure $siftUp(i : \mathbb{N})$
    assert the heap property holds except maybe for $j = i$
    if $i = 1 \vee h[\lfloor i/2 \rfloor] \leq h[i]$ then return
    assert the heap property holds except for $j = i$
    $swap(h[i], h[\lfloor i/2 \rfloor])$
    assert the heap property holds except maybe for $j = \lfloor i/2 \rfloor$
    $siftUp(\lfloor i/2 \rfloor)$
```

Correctness follows from the stated invariants.

Exercise 111. Show that the running time of $\mathit{siftUp}(n)$ is $\mathcal{O}(\log n)$ and hence an insert takes time $\mathcal{O}(\log n)$

A $\mathit{deleteMin}$ returns the contents of the root and replaces it by the contents of node n. Since $h[n]$ might be larger than $h[1]$ or $h[2]$, this manipulation may violate the heap property at positions 1 or 2. This possible violation is repaired using $\mathit{siftDown}$.

```
Function $\mathit{deleteMin}$ : $\mathit{Element}$
    assert $n > 0$
    $\mathit{result} = h[1]$ : $\mathit{Element}$
    $h[1] := h[n]$;   $n$--
    $\mathit{siftDown}(1)$
    return $\mathit{result}$
```

Procedure $\mathit{siftDown}(1)$ moves the new contents of the root down the tree until the heap property holds. More precisely, consider the path p starting at the root and always proceeding to a child with smaller key, cf. Figure 6.1; in the case of equal keys, the choice is arbitrary. We extend the path until all children (there may be zero, one, or two) have a key no larger than $h[1]$. We put $h[1]$ into this position and move all elements on path p up by one position. In this way, the heap property is restored. The strategy is most easily formulated as a recursive procedure. A call of procedure $\mathit{siftDown}(i)$ repairs the heap property in the subtree rooted at i, assuming that it holds already for the subtrees rooted at $2i$ and $2i + 1$. Let us say that the heap property holds in the subtree rooted at i if it holds for all proper descendants of i but not necessarily for i itself.

```
Procedure $\mathit{siftDown}(i : \mathbb{N})$
    assert the heap property holds for the subtrees rooted at $j = 2i$ and $j = 2i + 1$
    if $2i \leq n$ then                                        // $i$ is not a leaf
        if $2i + 1 > n \vee h[2i] \leq h[2i + 1]$ then $m := 2i$ else $m := 2i + 1$
        assert the sibling of $m$ does not exist or it has smaller priority than $m$
        if $h[i] > h[m]$ then                       // the heap property is violated
            $\mathit{swap}(h[i], h[m])$
            $\mathit{siftDown}(m)$
    assert heap property @ subtree rooted at $i$
```

Exercise 112. Our current implementation of $\mathit{siftDown}$ needs about $2 \log n$ element comparisons. Show how to reduce this to $\log n + \mathcal{O}(\log \log n)$. Hint: Determine the path p first and then use binary search on this path to find the proper position for $h[1]$. Section 6.5 has more on variants of $\mathit{siftDown}$.

We can obviously build a heap from n elements by inserting them one after the other in $\mathcal{O}(n \log n)$ total time. Interestingly, we can do better by establishing the heap property in a bottom-up fashion: $\mathit{siftDown}$ allows us to establish the heap property for a subtree of height $k + 1$ provided the heap property holds for its subtrees of height k. The following exercise asks you to work out the details of this idea.

Exercise 113 (*buildHeap*). Assume that we are given an arbitrary array $h[1..n]$ and want to establish the heap property on it by permuting its entries. Consider two procedures for achieving this:

```
Procedure buildHeapBackwards
    for $i := \lfloor n/2 \rfloor$ downto 1 do  $siftDown(i)$

Procedure $buildHeapRecursive(i : \mathbb{N})$
    if $4i \leq n$ then
        $buildHeapRecursive(2i)$
        $buildHeapRecursive(2i + 1)$
    $siftDown(i)$
```

1. Show that both $buildHeapBackwards$, and $buildHeapRecursive(1)$ establish the heap property everywhere.
2. Implement both algorithms efficiently and compare their running time for random integers and $n \in \left\{10^i : 2 \leq i \leq 8\right\}$. It will be important how efficiently you implement $buildHeapRecursive$. In particular, it might make sense to unravel the recursion for small subtrees.

*c) For large n, the main difference between the two algorithms are memory hierarchy effects. Analyze the number of I/O operations needed to implement the two algorithms in the external memory model from the end of Section 2.2. In particular, show that if we have block size B and a fast memory of size $M = \Omega(B \log B)$ then $buildHeapRecursive$ needs only $\mathcal{O}(n/B)$ I/O operations.

The following theorem summarizes our results on binary heaps.

Theorem 22. *With the heap implementation of non-addressable priority queues, creating an empty heap and finding* min *takes constant time, $deleteMin$ and $insert$ take logarithmic time $\mathcal{O}(\log n)$, and build takes linear time.*

Proof. The binary tree represented by an heap of n elements has depth $k = \lceil \log n \rceil$. $Insert$ and $deleteMin$ explore one root to leaf path and hence have logarithmic running time, min returns the contents of the root and hence takes constant time. Creating an empty heap amounts to allocating an array and therefore takes constant time. $Build$ calls $siftDown$ for 2^ℓ nodes of depth ℓ. Such a call takes time $O(k - \ell)$. Thus total time is

$$\mathcal{O}\left(\sum_{0 \leq \ell < k} 2^\ell (k - \ell)\right) = \mathcal{O}\left(2^k \sum_{0 \leq \ell < k} \frac{k - \ell}{2^{k-\ell}}\right) = \mathcal{O}\left(2^k \sum_{j \geq 1} \frac{j}{2^j}\right) = \mathcal{O}(n) \ .$$

The last equality uses Equation (A.14).

Heaps are the basis of *heapsort*. We first *build* a heap from the elements and then repeatedly perform $deleteMin$. Before the i-th $deleteMin$ operation the i-th smallest element is stored at the root $h[1]$. We swap $h[1]$ and $h[n + i + 1]$ and sift the new root down to its appropriate position. At the end, h stores the elements sorted in decreasing order. Of course, we can also sort in increasing order by using a *max-priority queue*, i.e., a data structure supporting the operations $insert$ and deleting the maximum.

Heaps do not immediately implement the data type addressable priority queue, since elements are moved around in the array h during insertion and deletion. Thus the array indices cannot be used as handles.

Exercise 114 (Addressable binary heaps). Extend heaps to an implementation of addressable priority queues. How many additional pointers per element do you need? There is a solution with two additional pointers per element.

***Exercise 115 (Bulk insertion)** Design an algorithm for inserting k new elements into an n element heap. Give an algorithm that runs in time $\mathcal{O}(k + \log n)$. Hint: Use a similar bottom-up approach as for heap construction.

6.2 Addressable Priority Queues

Binary heaps have a rather rigid structure. All n elements are arranged into a single binary tree of height $\lceil \log n \rceil$. In order to obtain faster implementations of operations $insert$, $decreaseKey$, $remove$, and $merge$ we now look at structures which are more flexible in two aspects: First, the single tree is replaced by a collection of trees, a forest. Each tree is still *heap-ordered*, i.e., no child is smaller than its parent. In other words, the sequence of keys along any root to leaf path is non-decreasing. Figure 6.4 shows a heap-ordered forest. Second, the elements of the queue are stored in *heap items* that have a persistent location in memory. Hence, pointers to heap items can serve as $handle$s to priority queue elements. The tree structure is explicitly defined using pointers between items.

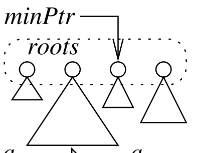
We will discuss several variants of addressable priority queues. We start with the common principles underlying all of them. Figure 6.3 summarizes the commonalities.

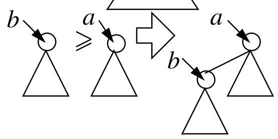
In order to keep track of the current minimum, we maintain the handle to the root containing it. We use $minPtr$ to denote this handle. The forest is manipulated using three simple operations: adding a new tree (and keeping $minPtr$ up to date), combining two trees into a single one, and cutting out a subtree making it a tree of its own.

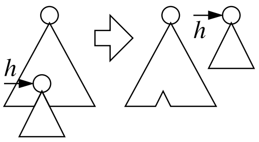
An $insert$ adds a new single node tree to the forest. So a sequence of n inserts into an initially empty heap will simply create n single node trees. The cost of an insert is clearly $\mathcal{O}(1)$.

A $deleteMin$ operation removes the node indicated by $minPtr$. This turns all children of the removed node into roots. We then scan the set of roots (old and new) to find the new minimum, a potentially very costly process. We also perform some rebalancing, i.e, we combine trees into larger ones. The details of this process distinguishes different addressable priority queues and is the key to efficiency.

```
Class AddressablePQ
    minPtr : Handle                        // root that stores the minimum
    roots : Set of Handle                  // pointers to tree roots
    Function min return element stored at minPtr

    Procedure link(a,b : Handle);   assert $a \leq b$
        remove $b$ from roots
        make $a$ the parent of $b$                              //

    Procedure combine(a,b : Handle)
        assert $a$ and $b$ are tree roots
        if $a \leq b$ then link$(a, b)$ else link$(b, a)$

    Procedure newTree(h : Handle)
        $roots := roots \cup \{i\}$
        if $h <$ min then $minPtr := i$

    Procedure cut(h : Handle)
        remove the subtree rooted at h from its tree            //
        newTree(h)

    Function insert(e : Element) : Handle
        $i$:=a Handle for a new Item storing $e$
        newTree($i$)
        return $i$

    Function deleteMin : Element
        $e$:= the Element stored in minPtr
        foreach child h of the root at minPtr do cut(h)         //
        perform some rebalancing         // uses combine
        return $e$

    Procedure decreaseKey(h : Handle, k : Key)
        change the key of h to k
        if $h$ is not a root then
            cut(h);   possibly perform some rebalancing

    Procedure remove(h : Handle)   key(h) := $-\infty$;   decreaseKey(h);   deleteMin

    Procedure merge(o : AddressablePQ)
        if $minPtr > o.minPtr$ then $minPtr := o.minPtr$
        $roots := roots \cup o.roots$
        $o.roots := \emptyset$;   possibly perform some rebalancing
```







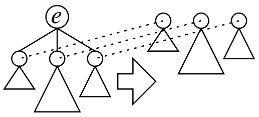


Fig. 6.3. Addressable priority queues.

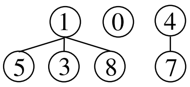


Fig. 6.4. A heap-ordered forest representing the set $\{0, 1, 3, 4, 5, 7, 8\}$.

We turn to $decreaseKey$ next. It is given a handle h and a new key k and decreases the key value of h to k. Of course, k must not be larger than the old key stored with h. Decreasing the information associated with h may destroy the heap property because h may now be smaller than its parent. In order to maintain the heap property, we cut the subtree rooted at h and turn h into a root. This sounds simple enough, but may create highly skewed trees. Therefore, some variants of addressable priority queues perform additional operations to keep the trees in shape.

The remaining operations are easy. We can $remove$ an item from the queue by first decreasing its key so that it becomes the minimum item in the queue and then perform a $deleteMin$. To merge a queue o into another queue we compute the union of $roots$ and $o.roots$. To update $minPtr$, it suffices to compare the minima of the merged queues. If the root sets are represented by linked lists, and no additional balancing is done, a merge needs only constant time.

In the sections to come we will discuss particular implementations of addressable priority queues.

6.2.1 Pairing Heaps

Pairing heaps [66][ps consistently insert refs early. Check: Move even more material from further findings?] use a very simple technique for rebalancing. Pairing heaps are efficient in practice, however a full theoretical analysis is missing. They rebalance only in $deleteMin$. If $\langle r_1, \ldots, r_k\rangle$ is the sequence of root nodes stored in $roots$ then $deleteMin$ $combine$s r_1 with r_2, r_3 with r_4, etc., i.e., the $roots$ are *paired*. Figure 6.5 gives an example. ⟸

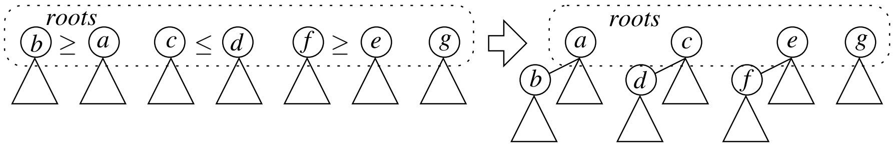


Fig. 6.5. The $deleteMin$ operation of pairing heaps combines pairs of root nodes.

Exercise 116 (Three pointer items). Explain how to implement pairing heaps using three pointers per heap item: One to the oldest child, one to the next younger sibling (if any), and one to the next older sibling. If there is no older sibling, the third pointer goes to the parent. Figure 6.8 gives an example.

***Exercise 117 (Two pointer items.)** Explain how to implement pairing heaps using two pointers per heap item: One to the oldest child and one to next older younger sibling. If there is no younger sibling, the second pointer goes to the parent. Figure 6.8 gives an example.

6.2.2 *Fibonacci Heaps

Fibonacci heaps [67] use more intensive balancing operations than pairing heaps. This paves the way to a theoretical analysis. In particular, we will get logarithmic amortized time for *remove* and *deleteMin* and worst case constant time for all other operations.

Each item of a Fibonacci heap stores four pointers that identify its parent, one child, and two siblings (cf. Figure 6.8). The children of each node form a doubly-linked circular list using the sibling pointers. The sibling pointers of the root nodes can be used to represent *roots* in a similar way. Parent pointers of roots and child pointers of leaf nodes have a special value, e.g., a null pointer.

In addition, every heap item contains a field *rank*. The *rank* of an item is the number of its children. In Fibonacci heaps, *deleteMin* links roots of equal rank r. The surviving root will then get rank $r + 1$. An efficient method to combine trees of equal rank is as follows. Let *maxRank* be an upper bound on the maximal rank of any node. We will prove below that *maxRank* is logarithmic in n. Maintain a set of buckets, initially empty and numbered from 0 to *maxRank*. Then scan the list of old and new roots. When a root of rank i is considered, inspect the i-th bucket. If the i-th bucket is empty then put the root there. If the bucket is non-empty then combine the two trees into one. This empties the i-th bucket and creates a root of rank $i + 1$. Try to throw the new tree into the i + 1st bucket. If it is occupied, combine .... When all roots have been processed in this way, we have a collection of trees whose roots have pairwise distinct ranks. Figure 6.6 gives an example.

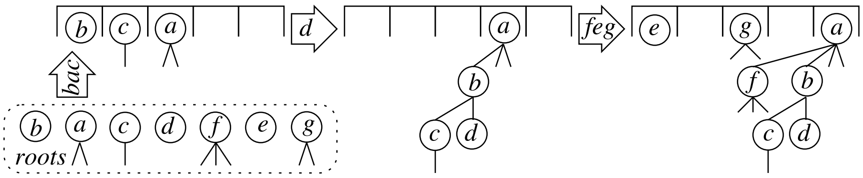


Fig. 6.6. An example for the development of the bucket array during execution of *deleteMin* of Fibonacci heaps. The arrows indicate the scanned roots. Note that scanning d leads to a cascade of three combines.

A *deleteMin* can be very expensive if there are many roots. For example, a *deleteMin* following n insertions has cost $\Omega(n)$. However, in an amortized sense, the cost of *deletemin* is $\mathcal{O}(maxRank)$. The reader must be familiar with the technique of amortized analysis before proceeding, see Section 3.3. For the amortized analysis we postulate that each root holds one token. Tokens pay for a constant amount of computing time.

Lemma 17. *The amortized complexity of deleteMin is* $\mathcal{O}(maxRank)$.

Proof. A *deleteMin* first calls *newTree* at most *maxRank* times (since the degree of the old minimum is bounded by *maxRank*) and then initializes an array of size

$maxRank$. Thus its running time is $\mathcal{O}(maxRank)$ and it needs to create $maxRank$ new tokens. The remaining time is proportional to the number of $combine$ operations performed. Each combine turns a root into a non-root and is paid for by the token associated with the node turning into a non-root.

How can we guarantee that $maxRank$ stays small? Let us consider a very simple situation first. Suppose that we perform a sequence of inserts followed by a single $deleteMin$. In this situation, we start with a certain number of single node trees and all trees formed by combining are so-called *binomial trees* as shown in Figure 6.7. The binomial tree B_0 consists of a single node and the binomial tree B_{i+1} is obtained by combining two copies of B_i. This implies that the root of B_i has rank i and contains exactly 2^i nodes. Thus the rank of a binomial tree is logarithmic in the size of the tree.

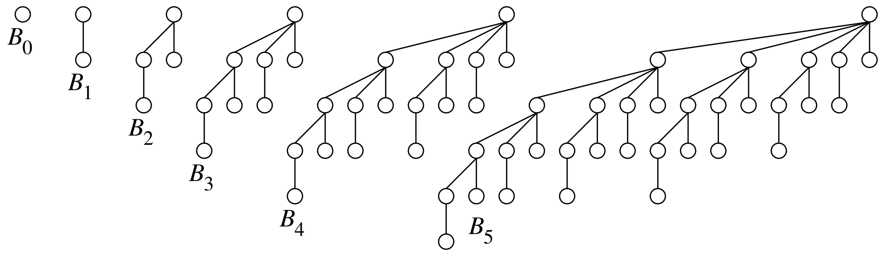


Fig. 6.7. The binomial trees of rank zero to five.

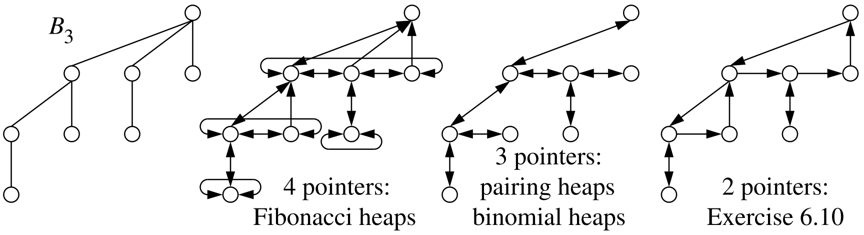


Fig. 6.8. Three ways to represent trees of nonuniform degree. The binomial tree of rank three, B_3, is used as an example.

Unfortunately, $decreaseKey$ may destroy the nice structure of binomial trees. Suppose item v is cut out. We now have to decrease the rank of its parent w. The problem is that the size of the subtrees rooted at the ancestors of w has decreased but their rank has not changed and hence we can no longer claim that size of a tree stays exponential in the rank of its root. Therefore, we have to perform some rebalancing

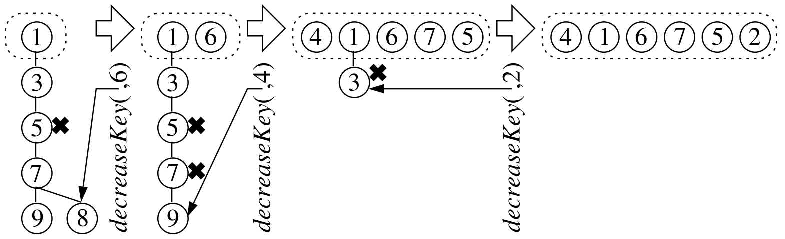


Fig. 6.9. An example for cascading cuts. Marks are drawn as crosses. Note that roots are never marked.

to keep the trees in shape. An old solution [189] is to keep all trees in the heap binomial. However, this causes logarithmic cost for a *decreaseKey*.

***Exercise 118 (Binomial heaps.)** Work out the details of this idea. Hint: Cut the following links: For each ancestor of v and including v cut the link to its parent. For each sibling of v of rank higher than v cut the link to its parent. Argue that the trees stay binomial and that the cost of *decreaseKey* is logarithmic.

Fibonacci heaps allow the trees to go out of shape but in a controlled way. The idea is surprisingly simple and is inspired by the amortized analysis of binary counters. We introduce an additional flag for each node. A node may be marked or not. Roots are never marked. In particular, when $\mathit{newTree}(h)$ is called in *deleteMin* it removes the mark from h (if any). Thus when *combine* combines two trees into one, neither node is marked.

When a non-root item x looses a child because *decreaseKey* is applied to the child, x is marked; this assumes that x is not already marked. When a marked node x loses a child, we cut x, remove the mark from x, and attempt to mark x's parent. If x's parent is already marked then .... This technique is called *cascading cuts*. In other words, suppose that we apply *decreaseKey* to an item v and that the k-nearest ancestors of v are marked. We turn v and the k-nearest ancestors of v into roots, unmark them, and mark the $k+1$st-nearest ancestor of v (if it is not a root). Figure 6.9 gives an example. Observe the similarity to carry propagation in binary addition.

For the amortized analysis, we postulate that each marked node holds two tokens and each root holds one token. Please check that this assumption does not invalidate the proof of Lemma 17.

Lemma 18. *The amortized complexity of decreaseKey is constant.*

Proof. Assume that we decrease the key of item v and that the k nearest ancestors of v are marked. Here $k \geq 0$. The running time of the operation is $O(1+k)$. Everyone of the k marked ancestors carries two tokens, i.e., we have a total of $2k$ tokens available. We create $k+1$ new roots and need one token for everyone of them. Also, we mark one unmarked node and need two tokens for it. Thus we need a total of $k+3$ tokens.

In other words $k - 3$ tokens are freed. They pay for all but $O(1)$ of the cost of *decreaseKey*. Thus the amortized cost of *decreaseKey* is constant.

How do cascading cuts affect the size of trees? We show that it stays exponential in the rank of the root. In order to do so we need some notation. Recall the sequence 0,1,1,2,3,5,8,... of Fibonacci numbers. They are defined by the recurrence $F_0 = 0$, $F_1 = 1$, and $F_i = F_{i-1} + F_{i-2}$ for $i \geq 2$. It is well-known that $F_{i+1} \geq (1 + \sqrt{5}/2)^i \geq 1.618^i$ for all $i \geq 0$.

Exercise 119. Prove $F_{i+1} \geq (1 + \sqrt{5}/2)^i \geq 1.618^i$ for all $i \geq 0$ by induction.

Lemma 19. *Let v be any item in a Fibonacci heap and let i be the rank of v. Then the subtree rooted at v contains at least F_{i+2} nodes. In a Fibonacci heap with n items all ranks are bounded by* $1.4404 \log n$.

Proof. Consider an arbitrary item v of rank i. Order the children of v by the time at which they were made children of v. Let w_j be the j-th child, $1 \leq j \leq i$. When w_j was made child of v, both nodes had the same rank. Also, since at least the nodes $w_1, \ldots, w_{j-1}$ were children of v at that time, the rank of v was at least $j - 1$ at the time when w_j was made a child of v. The rank of w_j has decreased by at most 1 since then because otherwise w_j would no longer be a child of v. Thus the current rank of w_j is at least $j - 2$.

We can now set up a recurrence for the minimal number S_i of nodes in a tree whose root has rank i. Clearly $S_0 = 1$, $S_1 = 2$, and $S_i \geq 2 + S_0 + S_1 + \cdots + S_{i-2}$. The last inequality follows from the fact that for $j \geq 2$, the number of nodes in the subtree with root w_j is at least S_{j-2}, and that we can also count the nodes v and w_1. The recurrence above (with = instead of $\geq$) generates the sequence 1, 2, 3, 5, 8,... which is identical to the Fibonacci sequence (minus its first two elements).

Let's verify this by induction. Let $T_0 = 1$, $T_1 = 2$, and $T_i = 2 + T_0 + \cdots + T_{i-2}$ for $i \geq 2$. Then, for $i \geq 2$, $T_{i+1} - T_i = 2 + T_0 + \cdots + T_{i-1} - 2 - T_0 - \cdots - T_{i-2} = T_{i-1}$, i.e., $T_{i+1} = T_i + T_{i-1}$. This proves $T_i = F_{i+2}$.

For the second claim, we observe that $F_{i+2} \leq n$ implies $i \cdot \log(1 + \sqrt{5}/2) \leq \log n$ which in turn implies $i \leq 1.4404 \log n$.

This concludes our treatment of Fibonacci heaps. We have shown:

Theorem 23. *The following time bounds hold for Fibonacci heaps: min, insert, and merge take worst case constant time; decreaseKey takes amortized constant time and remove and deleteMin take amortized time logarithmic in the size of the queue.*

Exercise 120. Describe a variant of Fibonacci heaps where all roots have distinct rank.

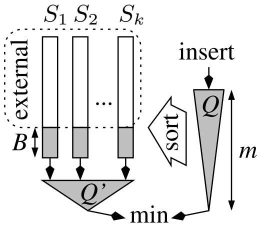


Fig. 6.10. Schematic view of an external memory priority queue.

6.*3 External Memory

We now go back to nonaddressable priority queues and consider their cache efficiency and I/O efficiency. A weakness of binary heaps is that the $siftDown$ operation goes down the tree in an unpredictable fashion. This leads to many cache faults and makes binary heaps prohibitively slow when they do not fit into the main memory. We now outline a data structure for (nonadressable) priority queues with more regular memory accesses. It is also a good example for a generally useful design principle: construction of a data structure out of simpler and known components and algorithms.

In this case, the components are internal memory priority queues, sorting, and multiway merging (see also Section 5.7). Figure 6.10 depicts the basic design. The data structure consists of two priority queues Q and Q' (e.g., binary heaps) and k sorted sequences S_1,..., S_k. Each element of the priority queue is either stored in the *insertion queue* Q, the *deletion queue* Q', or in one of the sorted sequences. The size of Q is limited to a parameter m. The *deletion queue* Q' stores the smallest element of each sequence together with the index of the sequence holding the element.

New elements are inserted into the insertion queue. If the insertion queue is full, it is first emptied. In this case, its elements form a new sorted sequence:

```
Procedure insert($e$ : $Element$)
    if $|Q| = m$ then    $k$++;   $S_k := sort(Q)$;   $Q := \emptyset$;   $Q'.insert(S_k.popFront)$
    $Q.insert(e)$
```

The minimum is stored either in Q or in Q'. If the minimum is in Q' and comes from sequence S_i, the next largest element from S_i is inserted into Q':

```
Function deleteMin
    if $\min Q \leq \min Q'$ then $e := Q.deleteMin$                // assume $\min \emptyset = \infty$
    else    $(e, i) := Q'.deleteMin$
            if $S_i \neq \langle\rangle$ then $Q'.insert((S_i.popFront, i))$
    return $e$
```

It remains to explain how the ingredients of our data structure are mapped to the memory hierarchy. The queues Q and Q' are stored in the internal memory. The size bound m for Q should be a constant fraction of the internal memory size M and a multiple of the block size B. The sequences S_i are largely kept externally. Initially, only the B smallest elements of S_i are kept in an internal memory buffer b_i. When the last element of b_i is removed, the next B elements of S_i are loaded. Note that we are effectively merging the sequences S_i. This is similar to our multiway merging algorithm from Section 5.7. Each inserted element is written to disk at most once and fetched back to internal memory at most once. Since all disk accesses are in units of at least a full block, the I/O requirement of our algorithm is at most n/B for n queue operations.

Our total requirement of internal memory is at most $m + kB + 2k$. This is below the total fast memory size M if $m = M/2$ and $k \leq \lfloor (M/2 - 2k)/B \rfloor \approx \frac{M}{2B}$. If there are many insertions, the internal memory may eventually overflow. However, the earliest this can happen is after $m(1 + \lfloor (M/2 - 2k)/B \rfloor) \approx \frac{M^2}{4B}$ insertions. For example, if we have 1 GByte of main memory, 8-byte elements, and 512 KByte disk blocks, we have $M = 2^{27}$ and $B = 2^{16}$ (measured in elements). We can then perform about 2^{36} insertions — enough for 128 GByte of data. Similar to external mergesort, we can handle larger amounts of data by performing multiple phases of multiway merging (e.g. [31, 154]). The data structure becomes considerably more complicated but it turns out that the I/O requirement for n insertions and deletions is about the same as for sorting n elements. An implementation of this idea is $2 - -3$ times faster than binary heaps for the hierarchy between cache and main memory [154]. There are also implementations for external memory [50].

6.4 Implementation Notes

There are various places where *sentinels* (cf. Chapter 3) can be used to simplify or (slightly) accelerate the implementation of priority queues. Since this may require additional knowledge about key values this could make a reusable implementation more difficult however.

- If $h[0]$ stores a Key no larger than any Key ever inserted into a binary heap then $siftUp$ need not treat the case $i = 1$ in a special way.
- If $h[n + 1]$ stores a Key no smaller than any Key ever inserted into a binary heap then $siftDown$ need not treat the case $2i + 1 > n$ in a special way. If such large keys are even stored in $h[n + 1..2n + 1]$ then the case $2i > n$ can also be eliminated.
- Addressable priority queues can use a special dummy item rather than a null pointer.

For simplicity we have formulated the operations $siftDown$ and $siftUp$ of binary heaps using recursion. It might be a bit faster to implement them iteratively instead.

Exercise 121. Give iterative versions of $siftDown$ and $siftUp$.

Some compilers do the recursion elimination for you.

As for sequences, memory management for items of addressable priority queues can be critical for performance. Often, a particular application may be able to do that more efficiently than a general-purpose library. For example, many graph algorithms use a priority queue of nodes. In this case, the item can be stored with the node.

There are priority queues that work efficiently for integer keys. It should be noted that these queues can also be used for floating point numbers. Indeed, the IEEE floating point standard has the interesting property that for any valid floating point numbers a and b, $a \leq b$ if an only $bits(a) \leq bits(b)$ where $bits(x)$ denotes the reinterpretation of x as an unsigned integer.

C++:

The STL class $priority\_queue$ offers non-addressable priority queues implemented using binary heaps. The external memory library STXXL [50] offers an external memory priority queue. LEDA implements a wide variety of addressable priority queues including pairing heaps and Fibonacci heaps.

Java:

The class $java.util.PriorityQueue$ supports addressable priority queues to the extent that $remove$ is implemented. However $decreaseKey$ and $merge$ are not supported. Also, it seems that the current implementation of $remove$ needs time $\Theta(n)$! JDSL offers an addressable priority queue $jdsl.core.api.PriorityQueue$ which is currently implemented as a binary heap.

6.5 Historical Notes and Further Findings

There is an interesting internet survey[1] on priority queues. It lists the applications (shortest) path planning (cf. Section 10), discrete event simulation, coding and compression, scheduling in operating systems, computing maximum flows, and branch-and-bound (cf. Section 12.4).

In Section 6.1 we have seen an implementation of $deleteMin$ by top-down search that needs about $2\log n$ element comparisons and a variant using binary search that needs only $\log n + \mathcal{O}(\log\log n)$ element comparisons. The latter is mostly of theoretical interest. Interestingly a very simple algorithm that first sifts the element down all the way to the bottom of the heap and than sifts it up again can be even better. When used for sorting, the resulting *Bottom-up heapsort* requires $\frac{3}{2}n\log n + \mathcal{O}(n)$ comparisons in the worst case and $n\log n + \mathcal{O}(1)$ in the average case [191, 61, 159]. While bottom-up heapsort is simple and practical, our own experiments indicate that it is not faster than the usual top-down variant (for integer keys). This surprised us. The explanation might be that the outcomes of the comparisons saved by the bottom-up variant are easy to predict. Modern hardware executes such predictable comparisons very efficiently (see [157] for more discussion).

The recursive $buildHeap$ routine from Exercise 113 is an example for a *cache-oblivious algorithm* [69]. The algorithm is efficient in the external memory model even though it does not explicitly use the block size or cache size.

[1] `http://www.leekillough.com/heaps/survey_results.html`

Pairing heaps [66] have amortized constant complexity for insert and merge [94] and logarithmic amortized complexity for $\mathit{deleteMin}$. The best analysis is due to Pettie [146]. Fredman [68] has given operation sequences consisting of $\mathcal{O}(n)$ insertions and $\mathit{deleteMin}$s and $\mathcal{O}(n \log n)$ $\mathit{decreaseKey}$s that require time $\Omega(n \log n \log \log n)$ for a family of addressable priority queues that includes all previously proposed variants of pairing heaps.

The family of addressable priority queues from Section 6.2 is large. Vuillemin [189] introduced binomial heaps and Fredman and Tarjan [67] invented Fibonacci heaps. Høyer describes additional balancing operations that are akin to the operations used for search trees. One such operation yields *thin heaps* [100] which have similar performance guarantees as Fibonacci heaps and do without parent pointer and mark bit. It is likely that thin heaps are faster in practice than Fibonacci heaps. There are also priority queues with worst case bounds asymptotically as good as the amortized bounds we have seen for Fibonacci heaps [30]. The basic idea is to tolerate violations of the heap property and to continuously invest some work reducing the violations. Another interesting variant are *fat heaps* [100].

Many applications only need priority queues for integer keys. For this special case there are more efficient priority queues. The best theoretical bounds so far are constant time $\mathit{decreaseKey}$ and insert and $\mathcal{O}(\log \log n)$ time for $\mathit{deleteMin}$ [182, 131]. Using randomization the time bound can even be reduced to $\mathcal{O}\left(\sqrt{\log \log n}\right)$ [196]. These algorithms are fairly complex. However, integer priority queues that also have the *monotonicity property* can be simple and practical. Section 10.3 gives examples. *Calendar queues* [33] are popular in the discrete event simulation community. They are a variant of the *bucket queues* described in Section 10.4.1. [verstehe den Text nicht ganz — ps: umformuliert] ⟸

7

Sorted Sequences

All of us spend a significant part of our time on searching and so do computers: they look up telephone numbers, balances of banking accounts, flight reservations, bills and payments, ... In many applications, we want to search dynamic collections of data. New bookings are entered into reservation systems, reservations are changed or cancelled, and bookings turn into actual flights. We have already seen one solution to the problem, namely hashing. It is often desirable to keep the dynamic collection sorted. The "manual data structure" used for this purpose is a filing card box. We can insert new cards at any position, we can remove cards, we can go through the cards in sorted order, and we can use some kind of binary search to find a particular card. Large libraries used to have filing card boxes with hundreds of thousands of cards.

Formally, we want to maintain a *sorted sequence*, i.e. a sequence of $\mathit{Element}$s sorted by their Key value, under the following operations:

$M.\mathit{locate}(k : \mathit{Key})$: **return** $\min \{e \in M : e \geq k\}$
$M.\mathit{insert}(e : \mathit{Element})$: $M := M \cup \{e\}$
$M.\mathit{remove}(k : \mathit{Key})$: $M := M \setminus \{e \in M : \mathit{key}(e) = k\}$

where M is the set of elements stored in the sequence. For simplicity, we assume that the elements have pairwise distinct keys. We will come to this assumption in Exercise 131. We will show that these operations can be implemented to run in time $\mathcal{O}(\log n)$ where n denotes the size of the sequence. How do sorted sequences compare with data structures known to us from previous chapters? They are more flexible than sorted arrays because they efficiently support insert and remove. They are slower but also more powerful than hash tables since locate also works when there is no element with key k in M. Priority queues are a special case of sorted sequences; they can only locate and remove the smallest element.

Our basic realization of sorted lists consists of a sorted doubly linked list with an additional navigation data structure supporting locate. Figure 7.1 illustrates this approach. Recall that a doubly linked list for n elements consists of $n + 1$ items, one for each element and one additional "header item". We use the header item to store a special key value $+\infty$ which is larger than all conceivable keys. We can then define the result of $\mathit{locate}(k)$ as the handle to the smallest list item $e \geq k$. If k is

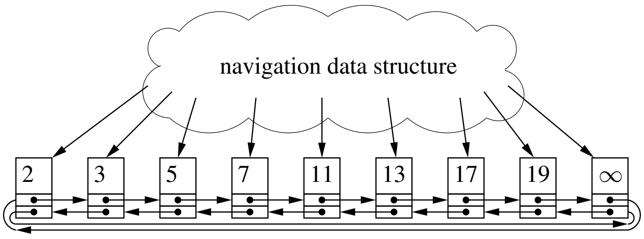


Fig. 7.1. A sorted sequence as a doubly linked list plus a navigation data structure.

larger than all keys in M, locate will return a handle to the dummy item. In Section 3.1.1 we learned that doubly linked lists support a large set of operations; most of them can also be implemented efficiently for sorted sequences. For example, we "inherit" constant time implementations for first, last, succ, and pred. We will see constant amortized time implementations for $\mathit{remove}(h : \mathit{Handle})$, $\mathit{insertBefore}$, and $\mathit{insertAfter}$, and logarithmic time algorithms for concatenating and splitting sorted sequences. The indexing operator $[\cdot]$ and finding the position of an element in the sequence also take logarithmic time. Before we delve into explaining the navigation data structure, let us look at some concrete applications of sorted sequences.

Best First Heuristics: Assume we want to pack items into a set of bins. The items arrive one at a time and have to be put into a bin immediately. Each item i has a weight $w(i)$ and each bin has a maximum capacity. The goal is to minimize the number of bins used. A successful heuristic solution for this problem is to put item i into the bin that fits best, i.e. whose remaining capacity is smallest among all bins with residual capacity being at least as large as $w(i)$ [42]. To implement this algorithm, we can keep the bins in a sequence s sorted by their residual capacity. To place an item, we call $s.\mathit{locate}(w(i))$, remove the bin we found, reduce its residual capacity by $w(i)$, and reinsert it into s. See also Exercise 214.

Sweep-Line Algorithms: Assume you have a set of horizontal and vertical line segments in the plane and want to find all points where two segments intersect. A sweep-line algorithm moves a vertical line over the plane from left to right and maintains the set of horizontal lines that intersect the sweep line in a sorted sequence s. When the left endpoint of a horizontal segment is reached, it is inserted into s and when its right endpoint is reached, it is removed from s. When a vertical line segment is reached at position x that spans the vertical range $[y, y']$, we call $s.\mathit{locate}(y)$ and scan s until we reach key y'.[1] All horizontal line segments discovered during this scan define an intersection. The sweeping algorithm can be generalized to arbitrary line segments [21], curved objects, and many other geometric problems[ps: cite sth ⟹ of recent results on curved objects?].

[1] This *range query* operation is also discussed in Section 7.3.

Data Base Indexes: A key problem in data bases is to make large collections of data efficiently searchable. A variant of the (a, b)-tree data structure explained in Section 7.2 is one of the most important data structures used in data bases.

The most popular navigation data structure are *search trees*. We will introduce search tree algorithms in three steps. As a warm-up, Section 7.1 introduces (unbalanced) *binary search trees* that support $locate$ in $\mathcal{O}(\log n)$ time under certain favorable circumstances. Since binary search trees are somewhat difficult to maintain under insertions and removals, we switch to a generalization, (a, b)-trees that allows search tree nodes of a larger degree. Section 7.2 explains how (a, b)-trees can be used to implement all three basic operations in logarithmic worst case time. In Section 7.3 we will augment search trees with additional mechanisms that support further operations.

7.1 Binary Search Trees

Navigating a search tree is a bit like asking your way around a foreign city. You ask a question, follow the advice, ask again, follow the advice, ..., until you reach your destination.

A *binary search tree* is a tree whose leaves store the elements of the sorted sequence in sorted order from left to right[2]. In order to locate a key k, we start at the root of the tree and follow the unique path to the appropriate leaf. How do we identify the correct path? To this end, the interior nodes of a search tree store keys that guide the search; we call these keys *splitter* keys. Every node in a binary search tree with $n \geq 2$ leaves has exactly two children, a *left* child and a *right* child. The splitter key s associated with a node has the property that all keys k stored in the left subtree satisfy $k \leq s$ and all keys k stored in the right subtree satisfy $k > s$.

With these definitions in place, it is clear how to identify the correct path when locating k. Let s be the splitter key of the current node. If $k \leq s$, go left. Otherwise, go right. Figure 7.2 gives an example. The length of the path from the root to a node is called its depth. The maximum depth of a leaf is the *height* of the tree. The height therefore tells us the maximum number of search steps needed to $locate$ a leaf.

Exercise 122. Prove that a binary search tree with $n \geq 2$ leaves can be arranged such that it has height $\lceil \log n \rceil$.

A search tree with height $\lceil \log n \rceil$ is called *perfectly balanced.* [ps inserted half sentence] The resulting logarithmic search time is a dramatic improvement, compared to the $\Omega(n)$ time needed for scanning a list. The bad news is that it is expensive to keep perfect balance when elements are inserted and removed. To understand this better, let us consider the "naive" insertion routine depicted in Figure 7.3. We locate the key k of the new element e before its successor e', insert e into the list, and then introduce a new node v with left child e and right child e'. The old parent u of e' now points to v. In the worst case, every insertion operation will locate a leaf at maximum ⟸

[2] There is also a variant of search trees where the elements are stored in all nodes of the tree.

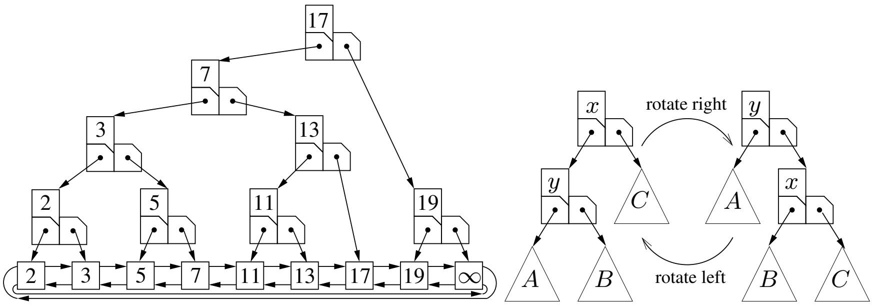


Fig. 7.2. Left: Sequence $\langle 2, 3, 5, 7, 11, 13, 17, 19\rangle$ represented by a binary search tree. In each node, we show the splitter key at the top and the pointers to the children at the bottom. Right: rotation of a binary search tree. The triangles indicate subtrees. Observe that the ancestor relationship between nodes x and y is interchanged.

depth so that the height of the tree increases every time. Figure 7.4 gives an example that shows that in the worst case the tree may degenerate to a list; we are back to scanning.

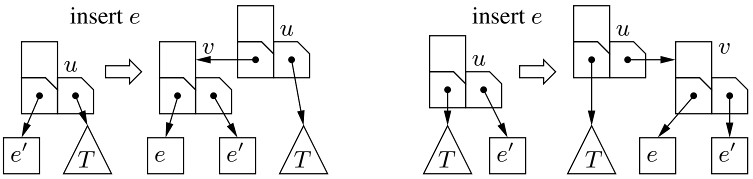


Fig. 7.3. Naive insertion into a binary search tree. A triangle indicates an entire subtree.

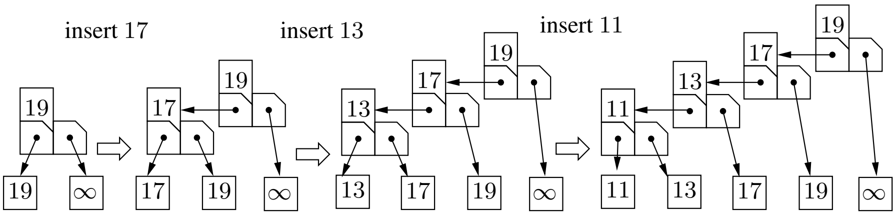


Fig. 7.4. Naively inserting sorted elements leads to a degenerate tree.

An easy solution to this problem is a healthy portion of optimism; perhaps it will not come to the worst. Indeed, if we insert n elements in *random* order, the expected height of the search tree is $\approx 2.99 \log n$ [53]. We will not prove this here but outline a connection to quicksort to make the result plausible. For example, consider how the tree from Figure 7.2 can be build using naive insertion[ps: reformulated sentence]. ⟸ We first insert 17; this splits the set into subsets $\{2, 3, 5, 7, 11, 13\}$ and $\{19\}$. Among the elements in the left subsets, we first insert 7; this splits the left subset into $\{2, 3, 5\}$ and $\{11, 13\}$. In quicksort terminology, we would say that 17 is chosen as the splitter in the top-level call and that 7 is chosen as the splitter in the left recursive call. So building a binary search tree and quicksort are completely analogous processes; the same comparisons are made, but at different times. Every element of the set is compared with 17. In quicksort, these comparisons take place when the set is split in the top-level call. In building a binary search tree, these comparisons take place when the elements of the set are inserted. So the comparison between 17 and 11 either takes place in the top-level call of quicksort or when 11 is inserted into the tree. We have seen (Theorem) that the expected number of comparisons in randomized quicksort is $O(n \log n)$. By the correspondence, the expected number of comparisons in building a binary tree by random insertions is also $O(n \log n)$. Thus any insertion requires $O(\log n)$ comparisons on average. Even more is true; with high probability each single insertion requires $O(\log n)$ comparisons and the expected height is $\approx 2.99 \log n$.

Can we guarantee that the height stays logarithmic [ps added:]also in the worst ⟸ case? Yes and there are many different ways to achieve logarithmic height. We will survey the techniques in Section 7.7 and discuss two solutions in detail in the next section. We will first discuss a solution which allows nodes of varying degree and then show how to balance binary trees by rotations.

Exercise 123. Figure 7.2 indicates how the shape of a binary tree can be changed by a transformation called *rotation*. Apply rotations to the tree in Figure 7.2 so that the node labelled 11 becomes the root of the tree.

Exercise 124. Explain how to implement an *implicit* binary search tree, i.e. the tree is stored in an array using the same mapping of tree structure to array positions as in the binary heaps discussed in Section 6.1. What are the advantages and disadvantages compared to a pointer-based implementation? Compare search in an implicit binary tree to binary search in a sorted array.

7.2 (a, b)-Trees

An (a, b)-tree is a search tree where all interior nodes, except for the root, have out-degree between a and b. Here a and b are constants. The root has degree one for a trivial tree with a single leaf. Otherwise, the root has degree between 2 and b. For $a \geq 2$ and $b \geq 2a - 1$, the flexibility in node degrees allows us to efficiently maintain the invariant that *all leaves have the same depth*, as we will see in a short while. Consider a node with out-degree d. With such a node we associate an array $c[1..d]$ of pointers to children and a sorted array $s[1..d-1]$ of $d-1$ splitter keys. The splitters guide the search. To simplify notation, we additionally define $s[0] = -\infty$

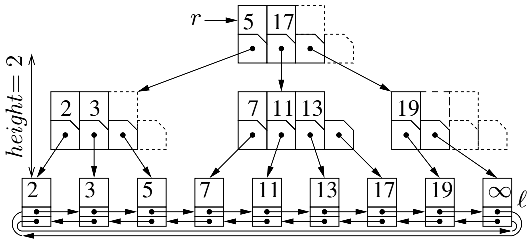


Fig. 7.5. Sequence $\langle 2, 3, 5, 7, 11, 13, 17, 19\rangle$ represented by a $(2, 4)$-tree. The tree has height 2.

and $s[d] = \infty$. The keys of the elements e contained in the i-th child $c[i]$, $1 \leq i \leq d$, lie between the $i - 1$-st splitter (exclusive) and the i-th splitter (inclusive), i.e. $s[i - 1] < \mathit{key}(e) \leq s[i]$. Figure 7.5 shows a $(2, 4)$-tree storing the sequence $\langle 2, 3, 5, 7, 11, 13, 17, 19\rangle$.

Lemma 20. *An (a, b)-tree for n elements has height at most* $1 + \left\lfloor \log_a \frac{n+1}{2} \right\rfloor$.

Proof. The tree has $n + 1$ leaves where the $+1$ accounts for the dummy leaf $+\infty$. If $n = 0$, the root has degree one and there is a single leaf. So assume $n \geq 1$. Let h be the height of the tree. Since the root has degree at least two and every other node has degree at least a, the number of leaves is at least $2a^{h-1}$. So $n + 1 \geq 2a^{h-1}$ or $h \leq 1 + \log_a(n + 1)/2$. Since the height is an integer, the bound follows.

Exercise 125. Prove that an (a, b)-tree for n elements has height at least $\lceil \log_b(n + 1)\rceil$. Prove that this bound and the bound given in Lemma 20 are tight.

Searching an (a, b)-tree is only slightly more complicated than searching a binary tree. Instead of performing a single comparison at a non-leaf node, we have to find the correct child among up to b choices. Using binary search, we need at most $\lceil \log b\rceil$ comparisons for each node on the search path. Figure 7.6 gives pseudocode for (a, b)-trees and the *locate* operation. Recall that we use the search tree as a way to locate items of a doubly linked list and that the dummy list item is considered to have key value ∞. This dummy item is the rightmost leaf in the search tree. Hence, there is no need to treat the special case of root degree 0 and the handle of the dummy item can serve as a return value when locating a key larger than all values in the sequence.

Exercise 126. Prove that the total number of comparisons in a search is bounded by $\lceil \log b\rceil\, (1 + \log_a(n + 1)/2)$. Assume $b \leq 2a$. Show that this is $O(\log b) + O(\log n)$. What is the constant in front of the $\log n$ term?

[ps:swapped floor and ceil in Fig. 7.7 to make compatible with pseudo ⟹ code] To *insert* an element e, we first descend the tree recursively to find the small-

```
Class ABHandle : Pointer to ABItem or Item
// an ABItem (Item) is an item in the navigation data structure (doubly linked list)

Class ABItem(splitters : Sequence of Key, children : Sequence of ABHandle)
    $d = |children| : 1..b$                                  // out-degree
    $s = splitters$ : Array $[1..b-1]$ of Key
    $c = children$ : Array $[1..b]$ of ABItem

    Function locateLocally($k$ : Key) : $\mathbb{N}$
        return $\min \{i \in 1..d : k \le s[i]\}$

    Function locateRec($k$ : Key, $h$ : $\mathbb{N}$) : Handle
        $i$:=locateLocally($k$)
        if $h = 1$ then return addressof $c[i]$
        else return $c[i] \rightarrow$locateRec($k$, $h-1$)

Class ABTree($a \ge 2 : \mathbb{N}$, $b \ge 2a-1 : \mathbb{N}$) of Element
    $\ell = \langle\rangle$ : List of Element
    $r$ : ABItem($\langle\rangle$, $\langle \ell.head \rangle$)
    height $= 1$ : $\mathbb{N}$

    // Locate the smallest Item with key $k' \ge k$
    Function locate($k$ : Key) : Handle return $r$.locateRec($k$, height)
```

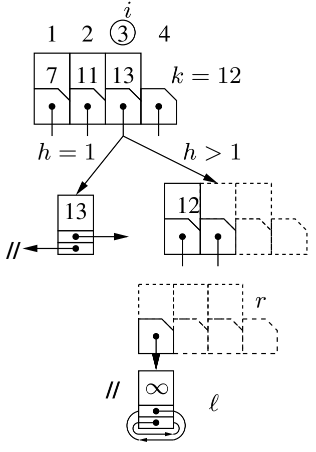


Fig. 7.6. (a, b)-trees. An ABItem is constructed from a sequence of keys and a sequence of handles to the children. The out-degree is the number of children. We allocate space for the maximum possible out-degree b. There are two functions local to ABItem: *locateLocally*(k) locates k among the splitters and *locateRec*(k, h) assumes that the ABItem has height h and descends h levels down the tree.
The constructor for ABTree creates a tree for the empty sequence. The tree has a single leaf, the dummy element, and the root has degree one. Locating a key k in an (a, b)-tree is solved by calling $r.$*locateRec*(k, h) where r is the root and h is the height of the tree.

Fig. 7.7. Node splitting: the node v of degree $b+1$ (here 5) is split into a node of degree $\lfloor (b+1)/2 \rfloor$ and a node of degree $\lceil (b+1)/2 \rceil$. The degree of the parent increases by one. The splitter key separating the two "parts" of v is moved to the parent.

est sequence element e' that is not smaller than e. If e and e' have equal keys, e' is replaced by e.

Otherwise, e is inserted into the sorted list ℓ before e'. If e' was the i-th child $c[i]$ of its parent node v then e will become the new $c[i]$ and $key(e)$ becomes the corresponding splitter element $s[i]$. The old children $c[i..d]$ and their corresponding splitters $s[i..d-1]$ are shifted one position to the right. If d was less than b, the incremented d is at most b and we are finished.

The difficult part is when a node v already had degree $d = b$ and now would get degree $b+1$. Let s' denote the splitters of this illegal node, c' its children, and u the parent of v (if it exists). The solution is to *split* v in the middle, see Figure 7.7.

More precisely, we create a new node t to the left of v and reduce the degree of v to $d = \lceil (b+1)/2 \rceil$ by moving the $b+1-d$ leftmost child pointers $c'[1..b+1-d]$ and the corresponding keys $s'[1..b-d]$. The old node v keeps the d rightmost child pointers $c'[b+2-d..b+1]$ and the corresponding splitters $s'[b+2-d..b]$.

The "leftover" middle key $k = s'[b+1-d]$ is an upper bound for the keys reachable from t. It and the pointer to t is needed in the predecessor u of v. The situation in u is analogous to the situation in v before the insertion: if v was the ith child of u, t is displacing it to the right. Now t becomes the i-th child and k is inserted as the i-th splitter. The addition of t as an additional child of u increases the degree of u. If the degree of u becomes $b+1$, we split u. The process continues until either some ancestor of v has room to accommodate the new child or until the root is split.

In the latter case, we allocate a new root node pointing to the two fragments of the old root. This is the only situation where the height of the tree can increase. In this case, the depth of all leaves increases by one, i.e. we maintain the invariant that all leaves have the same depth. Since the height of the tree is $\mathcal{O}(\log n)$ (cf. Exercise 125), we get a worst case execution time of $\mathcal{O}(\log n)$ for $insert$. Pseudocode is shown in Figure 7.8[3].

We still need to argue that $insert$ leaves us with a correct (a,b)-tree. When we split a node of degree $b+1$, we create nodes of degree $d = \lceil (b+1)/2 \rceil$ and $b+1-d$. Both degrees are clearly at most b. Also, $a \leq b+1-\lceil (b+1)/2 \rceil$ if $b \geq 2a-1$. Convince yourself that $b = 2a-2$ will not work.

$\Longrightarrow$ [todo:insertInlineBildchen ausrichten]

Exercise 127. It is tempting to streamline $insert$ by calling $locate$ to replace the initial descent of the tree. Why does this *not* work? Would it work if every node had a pointer to its parent?

We turn to operation $remove$. The approach is similar to what we already know from $insert$. We locate the element to be removed, remove it from the sorted list, and repair possible violations of invariants on the way back up. Figure 7.10 shows pseudocode and Figure 7.9 illustrates node fusing and balancing. When a parent u notices that the degree of its child $c[i]$ has dropped to $a-1$, it combines this child with one of its neighbors $c[i-1]$ or $c[i+1]$ to repair the invariant. There are two cases. If the neighbor has degree larger than a, we can *balance* the degrees by transferring some nodes from the neighbor. If the neighbor has degree a, balancing cannot help since both nodes together have only $2a-1$ children so that we cannot give a children to both of them. However, in this case we can *fuse* them to a single node since the requirement $b \geq 2a-1$ ensures that the fused node has degree at most b.

$\Longrightarrow$ To fuse a node $c[i]$ with its right neighbor $c[i+1]$,[ps: added comma] we concatenate their children arrays. To obtain the corresponding splitters, we need to place the splitter $s[i]$ from the parent between the splitter arrays. The fused node replaces $c[i+1]$, $c[i]$ can be deallocated, and $c[i]$ together with the splitter $s[i]$ can be removed from the parent node.

[3] From C++ we borrow the notation $C :: m$ to define a method m for class C.

```
// Example:
// $\langle 2,3,5\rangle.insert(12)$
**Procedure** $ABTree::insert(e : Element)$
    $(k,t){:=}r.insertRec(e, height, \ell)$
    **if** $t \neq$ **null then** // root was split
        $r{:=}new\ ABItem(\langle k\rangle, \langle r,t\rangle)$
        $height{+}{+}$

// Insert a new element into a subtree of height $h$.
// If this splits the root of the subtree,
// return the new splitter and subtree handle
**Function** $ABItem::insertRec(e : Element, h : \mathbb{N}, \ell : List$ **of** $Element) : Key \times ABHandle$
    $i := locateLocally(e)$
    **if** $h = 1$ **then**                                         // base case
        **if** $key(c[i] \to e) = key(e)$ **then**
            $c[i] \to e := e$
            **return** $(\perp,$ **null** $)$
        **else**
            $(k,t) := (key(e), \ell.insertBefore(e, c[i]))$      //
    **else**
        $(k,t){:=}c[i]{\to}insertRec(e, h-1, \ell)$
        **if** $t =$ **null then return** $(\perp,$ **null** $)$
    **endif**
    $s' := \langle s[1], \ldots, s[i-1], k, s[i], \ldots, s[d-1]\rangle$
    $c' := \langle c[1], \ldots, c[i-1], t, c[i], \ldots, c[d]\rangle$    //

    **if** $d < b$ **then**                 // there is still room here
        $(s,c,d) := (s',c',d+1)$
        **return** $(\perp,$ **null** $)$
    **else**                                // **split** this node
        $d := \lfloor (b+1)/2 \rfloor$
        $s := s'[b+2-d..b]$
        $c := c'[b+2-d..b+1]$                                     //
        **return** $(s'[b+1-d], newABItem(s'[1..b-d], c'[1..b+1-d]))$
```

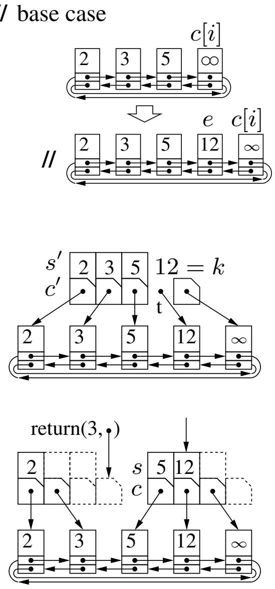


Fig. 7.8. Insertion into (a, b)-trees.

Fig. 7.9. Node balancing and fusing in (2,4)-trees: node v has degree $a-1$ (here 1). In the situation on the left, it has sibling of degree $a+1$ or more and we *balance* the degrees. In the situation on the right the sibling has degree a and we *fuse* v and its sibling. Observe how keys are moved. When two nodes are fused, the degree of the parent decreases.

Exercise 128. Suppose a node v has been produced by fusing two nodes as described above. Prove that the ordering invariant is maintained: An element[ps was: elements] e reachable through child $v.c[i]$ has key $v.s[i-1] < key(e) \leq v.s[i]$ for $1 \leq i \leq v.d$. $\Longrightarrow$

Balancing two neighbors is equivalent to first fusing them and then splitting the result as in operation $insert$.

Since fusing two nodes decreases the degree of their parent, the need to fuse or balance might propagate up the tree. If the degree of the root drops to one, we do one of two things. If the tree has height one and hence contains only a single element, there is nothing to do and we are finished. Otherwise, we deallocate the root and replace it by its sole child. The height of the tree decreases by one.

As for $insert$, the execution time of $remove$ is proportional to the height of the tree and hence logarithmic in the size of the sorted sequence. We summarize the performance of (a,b)-trees in the following theorem:

Theorem 24. *For any integers a and b with $a \geq 2$ and $b \geq 2a-1$, (a,b)-trees support operations insert, remove, and locate on sorted sequences of size n in time $\mathcal{O}(\log n)$.*

Exercise 129. Give a more detailed implementation of *locateLocally* based on binary search that needs at most $\lceil \log b \rceil$ comparisons. Your code should avoid both explicit use of infinite key values and special case treatments for extreme cases.

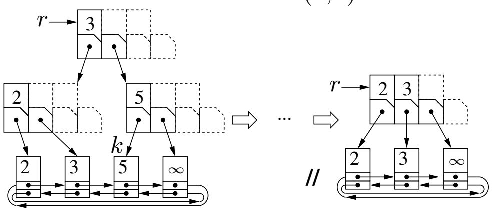
Exercise 130. Suppose $a = 2^k$ and $b = 2a$. Show that $(1+\frac{1}{k})\log n + 1$ element comparisons suffice to execute a *locate* operation in an (a,b)-tree. Hint: it is *not* quite sufficient to combine Exercise 125 with Exercise 129 since this would give you an additional term $+k$.

Exercise 131. Extend (a,b)-trees so that they can handle multiple occurences of[ps was: with] the same key. Hint: start by defining the semantics of $remove$. $\Longrightarrow$

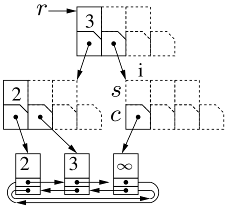
***Exercise 132 (Red-Black Trees)** A *red-black tree* is a binary search tree where the edges are colored either red or black. The *black depth* of a node v is the number of black edges on the path from the root to v. The following invariants have to hold:

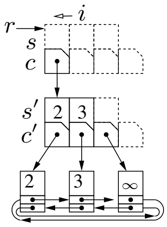
1. All leaves have the same black depth.
2. Edges into leaves are black.
3. No path from the root to a leaf contains two consecutive red edges.

```
//Example: $\langle 2,3,5\rangle$.remove(5)
Procedure ABTree::remove($k$ : $Key$) //
    $r.removeRec(k, height, \ell)$
    if $r.d = 1 \wedge height > 1$ then
        $r' := r;\ r := r'.c[1];$ dispose $r'$                    //
```



```
Procedure ABItem::removeRec($k : Key, h : \mathbb{N}, \ell$ : List of Element)
    i:=locateLocally(k)
    if $h = 1$ then                    // base case
        if $key(c[i] \to e) = k$ then // there is sth to remove
            $\ell.remove(c[i])$
            $removeLocally(i)$                                  //
    else
        $c[i] \to removeRec(e, h-1, \ell)$
        if $c[i] \to d < a$ then                               // invariant needs repair
            if $i = d$ then $i--$                  // make sure $i$ and $i+1$ are valid neighbors
            $s' := concatenate(c[i] \to s, \langle s[i]\rangle, c[i+1] \to s))$
            $c' := concatenate(c[i] \to c, c[i+1] \to c)$
            $d' := |c'|$
            if $d' \le b$ then                  // fuse
                $(c[i+1] \to s, c[i+1] \to c, c[i+1] \to d) := (s', c', d')$
                dispose $c[i]$;   $removeLocally(i)$                 //
            else                             // balance
                $m := \lceil d'/2 \rceil$
                $(c[i] \to s, c[i] \to c, c[i] \to d) := (s'[1..m-1], c'[1..m], m)$
                $(c[i+1] \to s,\quad c[i+1] \to c, c[i+1] \to d) :=$
                $(s'[m+1..d'-1],c'[m+1..d'], d'-m)$
                $s[i] := s'[m]$
```





```
//Remove the $i$-th child from an ABItem
Procedure ABItem::removeLocally($i : \mathbb{N}$)
    $c[i..d-1] := c[i+1..d]$
    $s[i..d-2] := s[i+1..d-1]$
    $d--$                                                    //
```

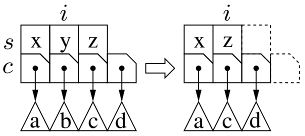


Fig. 7.10. Removal from an (a,b)-tree.

Fig. 7.11. The correspondance between (2,4)-trees and red-black trees. Nodes of degree 2, 3, and 4 as shown on the left correspond to the configurations on the right. Red edges are shown in bold.

Show that red-black trees and $(2,4)$-trees are isomorphic in the following sense: $(2,4)$-trees can be mapped to red-black trees by replacing nodes of degree three or four by two or three nodes connected by red edges respectively as shown in Figure 7.11. Red-black trees can be mapped to $(2,4)$-trees using the inverse transformation, i.e. components induced by red edges are replaced by a single node. Now explain how to implement $(2,4)$-trees using a representation as a red-black tree.[4] Explain how expanding, shrinking, splitting, merging, and balancing nodes of the $(2,4)$-tree can be translated into recoloring and rotation operations in the red-black tree. Colors should only be stored at the target nodes of the corresponding edges.

7.3 More Operations

Search trees support many operations in addition to $insert$, $remove$, and $locate$. We study them in two batches. In this section we will discuss operations directly supported by (a,b)-trees and in Section 7.5 we will discuss operations that require augmentation of the data structure.

min/max: The constant time operations *first* and *last* on a sorted list give us the smallest and largest element in the sequence in constant time. In particular, search trees implement *double-ended priority queues*, i.e. sets that allow locating and removing both the smallest and the largest element in logarithmic time. For example, in Figure 7.5, the header element of list ℓ gives us access to the smallest element 2 and to the largest element 19 via its $next$ and $prev$ pointers respectively.

$\Longrightarrow$ [todo: Ãijberall paragraph* → myparagraph]

Range queries: To retrieve all elements with keys in the range $[x,y]$,[ps added $\Longrightarrow$ comma] we first locate x and then traverse the sorted list until we see an element with a key larger than y. This takes time $\mathcal{O}(\log n + \text{output-size})$. For example, the range query $[4,14]$ applied to the search tree in Figure 7.5 will find the 5, subsequently outputs 7, 11, 13, and stops when it sees the 17.

Build/Rebuild: Exercise 133 asks you to give an algorithm that converts a sorted list or array into an (a,b)-tree in linear time. Even if we first have to sort an unsorted list, this operation is much faster than inserting the elements one by one. We also obtain a more compact data structure this way.

Exercise 133. Explain how to construct an (a,b)-tree from a sorted list in linear time. Which $(2,4)$-tree does your routine construct for the sequence $\langle 1..17\rangle$? Next, remove elements 4, 9, and 16.

* **Concatenation:** Two sorted sequences can be concatenated if the largest element of the first sequence is smaller than the smallest element in the second sequence. If sequences are represented as (a,b)-trees, two sequences s_1 and s_2 can be concatenated in time $\mathcal{O}(\log \max(|s_1|,|s_2|))$. First, we remove the dummy item from s_1 and concatenate the underlying lists. Next we fuse the root of one tree with an appropriate node of the other tree in such a way that the resulting tree remains sorted and balanced. More precisely, if $s_1.height \geq s_2.height$, we descend $s_1.height - s_2.height$ levels from the root of s_1 by following pointers to the rightmost children. The node v we reach is then fused with the root of s_2. The required new splitter key is the largest

[4] This may be more space efficient than a direct representation, in particular if keys are large.

key in s_1. If the degree of v now exceeds b, v is split. From that point, the concatenation proceeds like an *insert* operation propagating splits up the tree until the invariant is fulfilled or a new root node is created. The case $s_1.height < s_2.height$ is a mirror image. We descend $s_2.height - s_1.height$ levels from the root of s_2 by following pointers to the leftmost children, fuse .... The operation runs in time $\mathcal{O}(1 + |s_1.height - s_2.height|) = \mathcal{O}(\log n)$. Figure 7.12 gives an example.

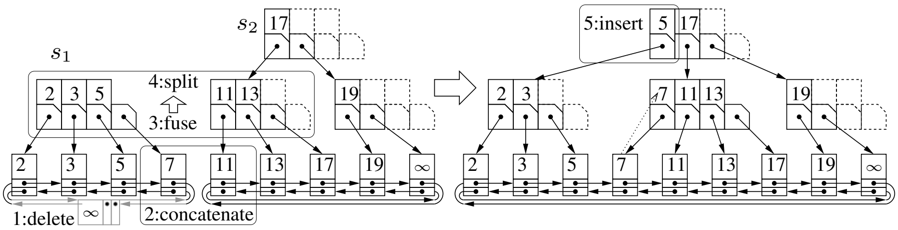


Fig. 7.12. Concatenating $(2,4)$-trees for $\langle 2,3,5,7\rangle$ and $\langle 11,13,17,19\rangle$.

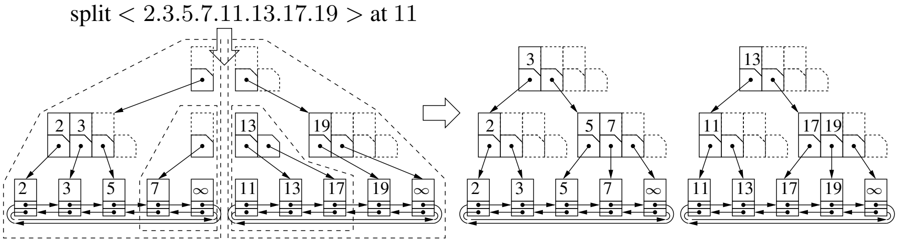


Fig. 7.13. Splitting the $(2,4)$-tree for $\langle 2,3,5,7,11,13,17,19\rangle$ from Figure 7.5 produces the subtrees shown on the left. Subsequently concatenating the trees surrounded by the dashed lines leads to the $(2,4)$-trees shown on the right side.

* **Splitting:** We show how to split a sorted sequence at a given element in logarithmic time. Consider sequence $s = \langle w, \ldots, x, y, \ldots, z\rangle$. Splitting s at y results in the sequences $s_1 = \langle w, \ldots, x\rangle$ and $s_2 = \langle y, \ldots, z\rangle$. We carry out the procedure as follows. Consider the path from the root to leaf y. We split each node v on this path into two nodes v_ℓ and v_r. Node v_ℓ gets the children of v that are to the left of the path and v_r gets the children that are to the right of the path. Some of these nodes may get no children. Each of the nodes with children can be viewed as the root of an (a,b)-tree. Concatenating the left trees and a new dummy sequence element yields the elements up to x. Concatenating $\langle y\rangle$ and the right trees produces the sequence of elements starting from y. We can do these $\mathcal{O}(\log n)$ concatenations in total time $\mathcal{O}(\log n)$ by exploiting the fact that the left trees have strictly decreasing height and the right trees have strictly increasing height. Let us look at the trees on the left in more detail. Let r_1, r_2

to r_k be the roots of the trees on the left and let h_1, h_2 to h_h be their heights. Then $h_1 \geq h_2 \geq \ldots \geq h_k$. We first concatenate r_{k-1} and r_k in time $\mathcal{O}(1 + h_{k-1} - h_k)$, then concatenate r_{k-2} with the result in time $\mathcal{O}(1 + h_{k-2} - h_{k-1})$, then concatenate r_{k-3} with the result in $\mathcal{O}(1 + h_{k-2} - h_{k-1})$, and so on. The total time needed for all concatenations is $\mathcal{O}\left(\sum_{1 \leq i < k}(1 + h_i - h_{i+1})\right) = \mathcal{O}(k + h_1 - h_k) = \mathcal{O}(\log n)$. Figure 7.13 gives an example.

Exercise 134. We glanced over one issue in the argument above. What is the height of the tree resulting from concatenating v_k to v_i. Show that the height is $h_i + \mathcal{O}(1)$.

Exercise 135. Explain how to delete a subsequence $\langle e \in s : \alpha \leq e \leq \beta \rangle$ from an (a, b)-tree s in time $\mathcal{O}(\log n)$.

7.4 Amortized Analysis of Update Operations

The best case time for an insertion or removal is considerably smaller than the worst case time. In the best case, we basically pay to locate the affected element, the update of the sequence, and the time for updating the bottommost internal node. The worst case is much slower. Split or fuse operations may propagate all the way up the tree.

Exercise 136. Give a sequence of n operations on $(2, 3)$-trees that requires $\Omega(n \log n)$ fusing and split operations.

We now show that the *amortized* complexity is basically equal to the best case if b is not at its minimum possible value but is at least $2a$. In Section 7.5.1 we will see variants of $insert$ and $remove$ that turn out to have constant amortized complexity in the light of the analysis below.

Theorem 25. *Consider an (a, b)-tree with $b \geq 2a$ that is initially empty. For any sequence of n insert or remove operations, the total number of split or fuse operations is $\mathcal{O}(n)$.*

Proof. We give the proof for $(2, 4)$-trees and leave the generalization to Exercise 137. We use the bank account method introduced in Section 3.3. Splits and fuse operations are paid for by tokens. They cost one token each. We charge two tokens to each $remove$ and $insert$ and claim that this suffices to pay for all $split$ and $fuse$ operations. In order to do the accounting, we associate the tokens with the nodes of the tree and show that the nodes can hold tokens according to the following table (*token invariant*):

degree	1	2	3	4	5
tokens	○○	○		○○	○○○○

Note that we have included the cases of degree 1 and 5 that occur during rebalancing. The purpose of splitting and fusing is to remove these exceptional degrees.

$\Longrightarrow$ [todo: redraw using tabular and latex picture]

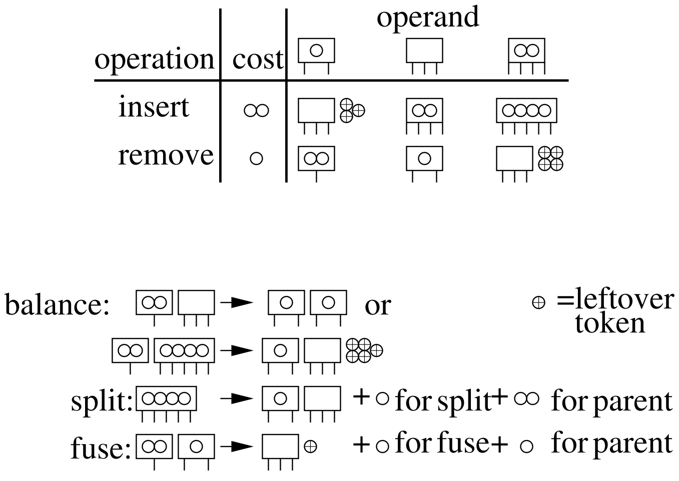


Fig. 7.14. The effect of (a, b)-tree operations on the token invariant. The upper part illustrates the addition or removal of a leaf. An insert is charged two tokens. When the leaf is added to a node of degree three or four, the two tokens are put on the node. When the leaf is added to a node of degree two, the two tokens are not needed and the token from the node is also freed. The lower part illustrates the use of the tokens in balance, split, and fuse operations.

Creating an empty sequence makes a list with one dummy item and a root of degree one. We charge two tokens to the *create* and put them on the root. Let us next look at insertions and deletions. They add or remove a leaf and hence increase or decrease the degree of a node immediately above leaf level. Increasing the degree of a node requires up to two additional tokens on the node (if the degree increases from 3 to 4 or from 4 to 5) and this is exactly what we charge to an insertion. If the degree grows from 2 to 3, we do not need additional tokens and we are overcharging the insertion; there is no harm in this. Similarly, reducing the degree by one, may require one additional token on the node (if the degree decreases from 3 to 2 or from 2 to 1) and this uses up one of the tokens charged to the removal. The other token we put aside for later use. So immediately after adding or removing a leaf, the token invariant is satisfied. We have also put one token aside in the case of a removal.

We next need to consider what happens during rebalancing. Figure 7.14 summarizes the discussion to follow graphically.

A *split* operation is performed on nodes of (temporary) degree five and results in a node of degree three and a node of degree two. It also increases the degree of the parent. The four tokens stored on the degree five node are spent as follows: one token pays for the *split*, one token is put on the new node of degree two, and two tokens are used for the parent node. Again, we may not need the additional tokens for the parent node; in this case, we discard them.

A *balance* operation takes a node of degree one and a node of degree three or four and moves one child from the high degree node to the node of degree one. If the high degree node has degree three, we have two tokens available to us and need two tokens; if the high degree node has degree four, we have four tokens available to us and need one token. In either case, the tokens available are sufficient to maintain the token invariant. We still need to pay for the operation itself. Here we use the token put aside. Observe, that a balance operation completes rebalancing after a removal and hence it is correct to put only one token aside.

A *fuse* operation fuses a degree one node with a degree two node into a degree three node and decreases the degree of the parent. We have three tokens available. We use one to pay for the operation and we use one to pay for the decrease of the degree of the parent. The third token is no longer needed and we discard it.

Let us summarize. We charge two tokens to each create, insert and remove. These tokens suffice to pay one token each for every split, fuse or balance. Thus n insert and remove operations can cause at most $2(n+1)$ rebalance operations.

***Exercise 137** Generalize the proof to arbitrary a and b with $b \geq 2a$. Show that n *insert* or *remove* operations cause only $\mathcal{O}(n/(b-2a+1))$ fuse or split operations.

***Exercise 138 (Weight-balanced trees [143])** Consider the following variant of (a, b)-trees: the node-by-node invariant $d \geq a$ is relaxed to the global invariant that the tree has at least $2a^{height-1}$ leaves. Remove does not perform any *fuse* or *balance* operations. Instead, the whole tree is rebuilt using the routine from Exercise 133 when the invariant is violated. Show that *remove* operations execute in $\mathcal{O}(\log n)$ amortized time.

7.5 Augmented Search Trees

We show that (a, b)-trees can support additional operations on sequences if we augment the data structure by additional information. However, augmentations come at a cost. They consume space and require time for keeping them up to date. Augmentations may also stand in each others' way. [ps dropped (where what is in each $\Longrightarrow$ others way in this exercise????): The following exercise gives an example.]

Exercise 139 (Reduction). Some operations on search trees can be carried out with the use of the navigation data structure alone and without the doubly linked list. Go through the operations discussed so far and discuss whether they require the *next* and *prev* pointers of linear lists. Range queries are a particular challenge.

7.5.1 Parent Pointers

Suppose we want to remove an element specified by the handle of a list item. In the basic implementation from Section 7.2, the only thing we can do is to read the key k of the element and call $remove(k)$. This would take logarithmic time for the search although we know from Section 7.4 that the amortized number of *fuse* operations required to rebalance the tree is constant. This detour is not necessary if each node

v of the tree stores a handle indicating its $parent$ in the tree (and perhaps an index i such that $v.parent.c[i] = v$).

Exercise 140. Show that in (a, b)-trees with parent pointers, the operations $remove(h : Item)$ and $insertAfter(h : Item)$ can be implemented to run in constant amortized time.

***Exercise 141 (Avoiding Augmentation)** Outline the implementation of a class $ABTreeIterator$ that represents a position in a sorted sequence in an ABTree *without* parent pointers. Creating an iterator I works like *search* and may take logarithmic time. The class should support operations *remove*, *insertAfter*, and operations for moving backward and forward in the host sequence by one position. All these operations should use constant amortized time. Hint: you may need a logarithmic amount of internal state.

***Exercise 142 (Finger Search)** Augment search trees such that searching can profit from a "hint" given in the form of the handle of a *finger element* e'. If the sought element has rank r and the finger element e' has rank r', the search time should be $\mathcal{O}(\log |r - r_0|)$. Hint: One solution links all nodes at each level of the search tree into a doubly linked list.

***Exercise 143 (Optimal Merging)** Explain how to use finger search to implement merging of two sorted sequences in time $\mathcal{O}\big(n \log \frac{m}{n}\big)$ where n is the size of the shorter sequence and m is the size of the longer sequence.

7.5.2 Subtree Sizes

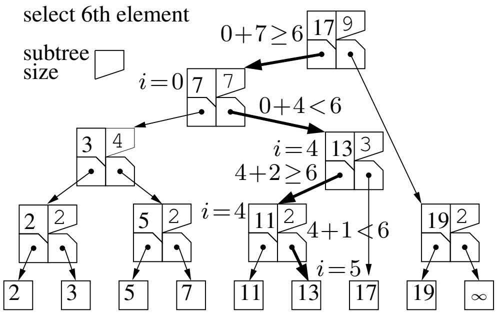


Fig. 7.15. Selecting the 6th smallest element from $\langle 2, 3, 5, 7, 11, 13, 17, 19\rangle$ represented by a binary search tree. The fat arrows indicate the search path.

Suppose every non-leaf node t of a search tree stores its $size$, i.e. $t.size$ is the number of leaves in the subtree rooted at t. Then the k-th smallest element of the sorted sequence can be selected in time proportional to the height of the tree. For simplicity, we describe this for binary search trees. Let t denote the current search tree node which is initialized to the root. The idea is to descend the tree while maintaining the invariant that the k-th element is contained in the subtree rooted at t. We also maintain the number i of [ps dropped: the] elements that are to the *left* of t. ⟸ Initially, $i = 0$. Let i' denote the size of the left subtree of t. If $i + i' \geq k$ then we set t to its left successor. Otherwise, t is set to its right successor and i is increased by i'. When a leaf is reached, the invariant ensures that the k-th element is reached. Figure 7.15 gives an example.

Exercise 144. Generalize the above selection algorithm to (a, b)-trees. Develop two variants. One that needs time $\mathcal{O}(b \log_a n)$ and stores only the subtree size. Another variant needs only time $\mathcal{O}(\log n)$ and stores $d - 1$ sums of subtree sizes in a node of degree d.

Exercise 145. Explain how to determine the rank of a sequence element with key k in logarithmic time.

Exercise 146. A colleague suggests supporting both logarithmic selection time and constant amortized update time by combining the augmentations from Sections 7.5.1 and 7.5.2. What will go wrong?

7.6 Implementation Notes

Our pseudocode for (a, b)-trees is close to an actual implementation in a language such as C++ except for a few oversimplifications. The temporary arrays s' and c' in procedures $insertRec$ and $removeRec$ can be avoided by appropriate case distinctions. In particular, a balance operation will not require calling the memory manager. A split operation of a node v might get slightly faster if v keeps the left half rather than the right half. We did not formulate it this way because then the cases of inserting a new sequence element and splitting a node are no longer the same from the point of view of their parent.

For large b, *locateLocally* should use binary search. For small b, linear search ⟹ might be better[ps was: applicable]. Furthermore, we might want to have a specialized implementation for small, fixed values of a and b that *unrolls*[5] all the inner loops. Choosing b to be a power of two might simplify this task.

Of course, the crucial question is how a and b should be chosen. Let us start with the cost of $locate$. There are two kinds of operations that dominate the execution time of $locate$: element comparisons (because of their inherent cost and because they may cause branch mispredictions[6]) and pointer dereferences (because they may cause cache faults). Exercise 130 indicates that element comparisons are minimized

[5] *Unrolling* a loop "**for** $i := 1$ **to** K **do** $body_i$" means replacing it by the *straight line program* "$body_1$,...,$body_K$". This saves the overhead for loop control and may give other opportunities for simplifications.

[6] Modern microprocessors attempt to execute many (up to a hundred or so) instructions in parallel. This works best if they come from a linear, predictable sequence of instructions. The branches in search trees have a 50 % chance of going either way *by design* and hence are likely to disrupt this scheme. This leads to large delays when many partially executed instructions have to be discarded.

by choosing a as a large power of two and $b = 2a$. Since the number of pointer dereferences is proportional to the height of the tree (cf. Exercise 125), large values of a are also good for this measure. Taking this reasoning to the extreme, we would obtain best performance for $a \geq n$, i.e. a single sorted array. This is not astonishing. We have concentrated on searches and static data structures are best if updates are neglected.

Insertions and deletions have the amortized cost of one $locate$ plus a constant number of node reorganizations (split, balance, or fuse) with cost $\mathcal{O}(b)$ each. We get logarithmic amortized cost for update operations if[ps was for] $b = \mathcal{O}(\log n)$. A ⟸ more detailed analysis 137 would reveal that increasing b beyond $2a$ makes split and fuse operations less frequent and thus saves expensive calls to the memory manager associated with them. However, this measure has a slightly negative effect on the performance of $locate$ and it clearly increases *space consumption*. Hence, b should remain close to $2a$.

Finally, let us have a closer look at the role of cache faults. The cache can hold $\Theta(M/b)$ nodes. These are most likely to be nodes close to the root since these are visited more often than deeper nodes. In a first approximation, the top $\log_a(M/b)$ levels of the tree are stored in the cache. Below this level, every pointer dereference is associated with a cache miss, i.e. we will have about $\log_a(bn/\Theta(M))$ cache misses in a cache of size M. Since cache blocks of processor caches start at addresses that are a multiple of the block size, it makes sense to *align* the starting address of search tree nodes to a cache block, i.e. to make sure that they also start at an address that is a multiple of the block size. Note that (a, b)-trees might well be more efficient than binary search for large data sets because we may save a factor $\log a$ cache misses.

Very large search trees are stored on disks. Indeed, under the name *BTrees*[check B+ Trees???] [14], (a, b)-trees are the working horse of indexing data structures in ⟸ data bases. In that case, internal nodes have a size of several KBytes. Furthermore, the linked list items are also replaced by entire data blocks that store between a' and b' elements for appropriate values of a' and b' (See also Exercise 47). These leaf blocks will then also be subject to splitting, balancing and fusing operations. For example, assume we have $a = 2^{10}$, the internal memory is large enough (a few MBytes) to cache the root and its children, and data blocks store between 16 and 32 KBytes of data. Then two disk accesses are sufficient to $locate$ any element in a sorted sequence that takes 16 GBytes of storage. Since putting elements into leaf blocks dramatically decreases the total space needed for the internal nodes and makes it possible to perform very fast range queries, this measure can also be useful for a cache efficient internal memory implementation. However, note that update operations may now move an element in memory and thus will invalidate element handles stored outside the data structure. There are many more tricks for implementing (external memory) (a, b)-trees. We refer the reader to [78] and [134, Chapters 2,14] for overviews. A good free implementation of BTrees is available in STXXL [50].

Even from the augmentations discussed in Section 7.5 and the implementation tradeoffs discussed here, you have hopefully learned that *the* optimal implementation of sorted sequences does not exist but depends on the hardware and the operation mix relevant for the actual application. We believe, that (a, b)-trees with $b = 2^k = 2a =$

$\mathcal{O}(\log n)$ augmented with parent pointers and a doubly linked list of leaves are a sorted sequence data structure that supports a wide range of operations efficiently.

Exercise 147. What choice of a and b in (a,b)-trees guarantees that the number of I/O operations required for insert, remove, or locate is $\mathcal{O}\big(\log_B \frac{n}{M}\big)$? How many I/O are needed to *build* an n elements (a,b)-tree using the external sorting algorithm from Section 5.7 as a subroutine? Compare this with the number of I/Os needed for building the tree naively using insertions. For example, try $M = 2^{29}$ byte, $B = 2^{18}$ byte[7] , $n = 2^{32}$, and elements having 8 byte keys and 8 bytes of associated information.

C++: The STL has four container classes set, map, $\mathit{multiset}$, and $\mathit{multimap}$ for sorted sequences. The prefix *multi* means that there may be several elements with the same key. *Map*s offer the interface of an associative array (see also Chapter 4). For example, $\mathit{someMap}[k] := x$ inserts or updates the element with key k and associated information x.

Exercise 148. Explain how our implementation of (a,b)-trees can be generalized to implement multisets. Elements with identical keys should be treated last-in-first-out, i.e. $\mathit{remove}(k)$ should remove the least recently inserted element with key k.

The most widespread implementation of sorted sequences in STL uses a variant of red-black trees with parent pointers where elements are stored in all nodes rather than only in the leaves. None of the STL data types supports efficient splitting or concatenation of sorted sequences.

LEDA offers a powerful interface $\mathit{sortseq}$ that supports all important (and many not so important) operations on sorted sequences including finger search, concatenation, and splitting. Using an implementation parameter, there is a choice between (a,b)-trees, red-black trees, randomized search trees, weight-balanced trees, and skip lists.

⟹ **Java:** The Java library $\mathit{java.util}$[check wording/typesetting in other chapters] offers the interface classes $\mathit{SortedMap}$ and $\mathit{SortedSet}$ which correspond to the STL classes set and map respectively. The corresponding implementation classes $\mathit{TreeMap}$ and $\mathit{TreeSet}$ are based on red-black trees.

7.7 Historical Notes and Further Findings

There is an entire zoo of sorted sequence data structures. Just about any of them will do, if you just want to support insert, remove, and locate in logarithmic time. Performance differences for the basic operations are often more dependent on implementation details than on fundamental properties of the underlying data structures. The differences show up in the additional operations.

[7] We are committing a slight oversimplification here since in practice one will use much smaller block sizes for organizing the tree than for sorting.

The first sorted sequence data structure to support $insert$, $remove$, and $locate$ in logarithmic time were AVL trees [3]. AVL trees are binary search trees which maintain the invariant that the heights of the subtrees of a node differ by one [ask google whether “at the most” is really good English]at the most. Since this is a strong ⟸ balancing condition, $locate$ is probably a bit faster than in most competitors. On the other hand, AVL trees do *not* support constant amortized update costs. Another small disadvantage is that storing the heights of subtrees costs additional space. In comparison, red-black trees have slightly higher costs for $locate$ but they have faster updates and the single color bit can often be squeezed in somewhere. For example, pointers to items will always store even addresses so that their least significant bit could be diverted to storing color information.

$(2, 3)$-trees were introduced in [5]. The generalization to (a, b)-trees and the amortized analysis of Section **??** comes from [93]. There it is also shown that the total number of splitting and fusing operations at the nodes of a certain height decreases exponentially in the height.

Splay trees [173] and some variants of randomized search trees [165] even work without any additional information besides one key and two successor pointers. A more interesting advantage of these data structures is their *adaptability* to nonuniform access frequencies. If an element e is accessed with probability p, these search trees will be reshaped over time to allow an access to e in time $\mathcal{O}(\log(1/p))$. This can be shown to be asymptotically optimal for any comparison-based data structure. However, this property leads to improved running time only for quite skewed access patterns because of the large constants.

Weight-balanced trees [143] balance the size of the subtrees instead of the height. They have the advantages that a node of weight w (= number of leaves of its subtree) is only rebalanced after $\Omega(w)$ insertions or deletions passing through it [27] and [121, TODO]. [remember above TODO] ⟸

There are so many *search tree* data structures for *sorted sequences* that these two terms are sometimes used as synonyms. However, there are equally interesting data structures for sorted sequences that are *not* based on search trees. Sorted arrays are a simple *static* data structure. Sparse tables [95] are an elegant way to make sorted arrays dynamic. The ideas is to accept some empty cells to make insertion easier. [18] extends sparse tables to a data structure which is asymptotically optimal in an amortized sense. Moreover, this data structure is a crucial ingredient for a sorted sequence data structure [18] which is *cache oblivious* [69], i.e. cache efficient on any two levels of a memory hierarchy without even knowing the size of caches and cache blocks. The other ingredient is oblivious *static* search trees [69]; these are perfectly balanced binary search trees stored in an array such that any search path will exhibit good locality in any cache. We describe the *van Emde Boas layout* used for this purpose for the case that there are $n = 2^{2^k}$ leaves for some integer k: store the top 2^{k-1} levels of the tree in the beginning of the array. After that, store the 2^{k-1} subtrees of depth 2^{k-1} allocating consecutive blocks of memory for them. Recursively allocate the resulting $1 + 2^{k-1}$ subtrees. At least static cache-oblivious search trees are practical in the sense that they can outperform binary search in a sorted array.

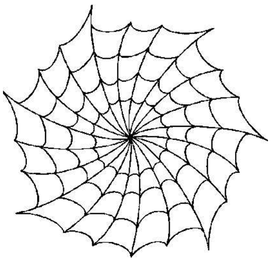
Skip lists [149] are based on another very simple idea. The starting point is a sorted linked list ℓ. The tedious task of scanning ℓ during $locate$ can be accelerated by producing a shorter list ℓ' that only contains some of the elements in ℓ. If corresponding elements of ℓ and ℓ' are linked, it suffices to scan ℓ' and only descend to ℓ when approaching the searched element. This idea can be iterated by building shorter and shorter lists until only a single element remains in the highest level list. This data structure supports all important operations efficiently in an expected sense. Randomness comes in because the decision which elements to lift to a higher level list is made randomly. Skip lists are particularly well suited for supporting finger search.

Yet another family of sorted sequence data structures comes into play when we no longer consider keys as atomic objects that can only be compared. If keys are numbers in binary representation, we obtain faster data structures using ideas similar to the fast integer sorting algorithms from Section 5.6. For example, sorted sequences with w bit integer keys support all operations in time $\mathcal{O}(\log w)$ [186, 125]. At least for 32 bit keys these ideas bring considerable speedup also in practice [49]. Not astonishingly, string keys are important. For example, suppose we want to adapt (a, b)-trees to use variable length strings as keys. If we want to keep a fixed size for node objects, we have to relax the condition on the minimal degree of a node. Two ideas can be used to avoid storing long string keys in many nodes: *common prefixes* of keys need to be stored only once, often in the parent nodes. Furthermore, it suffices to store the *distinguishing prefixes* of keys in inner nodes, i.e. just enough characters to be able to distinguish different keys in the current node [82]. Taking these ideas to the extreme results in *tries* [64], a search tree data structure specifically designed for strings keys: tries are trees whose edges are labelled by characters or strings. The characters along a root leaf path represent a key. Using appropriate data structures for the inner nodes, a trie can be searched in time $\mathcal{O}(s)$ for a string of size s.

We will close with three interesting generalizations of sorted sequences. The first generalization is *multi-dimensional objects* such as intervals or points in d-dimensional space. We refer to textbooks on geometry for this wide subject [48]. The second generalization is *persistence*. A data structure is persistent if it supports non-destructive updates. For example, after the insertion of an element, there are two versions of the data structure, the one before the insertion and the one after the insertion. Both can be searched [60]. The third generalization is *searching many sequences* [38, 37, 126]. In this setting there are many sequences and searches need to locate a key in all of them or a subset of them.

8

Graph Representation



Scientific results are mostly available in the form of articles in journals, conference proceedings, and on various web resources. These articles are not self-contained but they cite previous articles with related content. However, when you read an article from 1975 with an interesting partial result, you often ask yourselves what is the current state of the art. In particular, you would like to know which newer articles cite the old article. Projects like Google Scholar provide this functionality by analyzing the reference section of articles and by building a database of articles that efficiently supports looking up articles citing a given article.

We can easily model this situation by a directed graph. The graph has a node for each article and an edge for each citation. An edge (u, v) from article u to article v means u cites v. In this terminology, every node (= article) stores all its outgoing edges (= the articles cited by it) but not the incoming edges (the articles citing it). If every node would also store the incoming edges, it would be easy to find the citing articles. A main task of Google Scholar is to construct the reversed edges. The example shows that the cost of even a very basic elementary operation on graphs, namely finding all edges entering a particular node, depends heavily on the representation of the graph. If the incoming edges are stored explicitly, the operation is easy, if the incoming edges are not stored, the operation is non-trivial.

In this chapter, we will give an introduction to the various possibilities of representing graphs in a computer. We mostly focus on directed graphs and assume that an undirected graph $G = (V, E)$ is represented in the same way as the (bi)directed graph $G' = (V, \bigcup_{\{u,v\} \in E} \{(u, v), (v, u)\})$. Figure 8.1 illustrates the concept of a bidirected graph. Most of the presented data structures also allow us to represent parallel edges and self-loops. We start with a survey of the operations that we may want to support.

Accessing associated information: Given a node or an edge, we frequently want to access information associated with it, e.g., the weight of an edge or the distance of a node. In many representations, nodes and edges are objects and we can directly store this information as a member of these objects. If not otherwise mentioned, we assume that $V = 1..n$ so that information associated with nodes can be stored in arrays. When all else fails, we can always store node or edge information in a hash table. Hence, accesses can be implemented to run in constant time. In the remainder of this book we abstract from the different options for realizing access by using data types $\mathit{NodeArray}$ and $\mathit{EdgeArray}$ to indicate an array-like data structure that can be indexed by nodes or edges, respectively.

Navigation: Given a node, we want to access its outgoing edges. It turns out that this operation is at the heart of most graph algorithms. As we have seen in the scientific article example, we sometimes also want to know the incoming edges.

Edge Queries: Given a pair of nodes (u,v), we may want to know whether this edge is in the graph. This can always be implemented using a hash table but we may want to have something even faster. A more specialized but important query is to find the *reverse edge* (v,u) of a directed edge $(u,v) \in E$ if it exists. This operation can be implemented by storing additional pointers connecting edges with their reversal.

Construction, Conversion and Output: The representation most suitable for the algorithmic problem at hand is not always the representation given initially. This is not a big problem since most graph representations can be translated into each other in linear time.

Update: Sometimes we want to add or remove nodes or edges. For example, the description of some algorithms is simplified if a node is added from which all other nodes can be reached (e.g. Figure 10.10).

8.1 Unordered Edge Sequences

Perhaps the simplest representation of a graph is an unordered sequence of edges. Each edge contains a pair of node indices and possibly associated information such as an edge weight. Whether these node pairs represent directed or undirected edges is merely a matter of interpretation. Sequence representation is often used for input and output. It is easy to add edges or nodes in constant time. However, many other operations, in particular navigation, take time $\Theta(m)$ which is forbiddingly slow. Only few graph algorithms work well with the edge sequence representation, most algorithms require easy access to the edges incident to any given node. Then the ordered representations discussed in the following sections are appropriate.[unignore ref to
$\Longrightarrow$ Kruskal?]

8.2 Adjacency Arrays — Static Graphs

To support easy access to the edges leaving any particular node, we can store the edges leaving any node in an array. If no additional information is stored with edges, this array would just contain the indices of the target nodes. If the graph is *static*, i.e., does not change over time, we can concatenate all these little arrays into a single edge array E. An additional array V stores the starting positions of the sub-arrays, i.e., for any node v, $V[v]$ is the index in E of the first edge out of V. It is convenient to add a dummy entry $V[n+1]$ with $V[n+1] = m+1$. The edges out of any node v

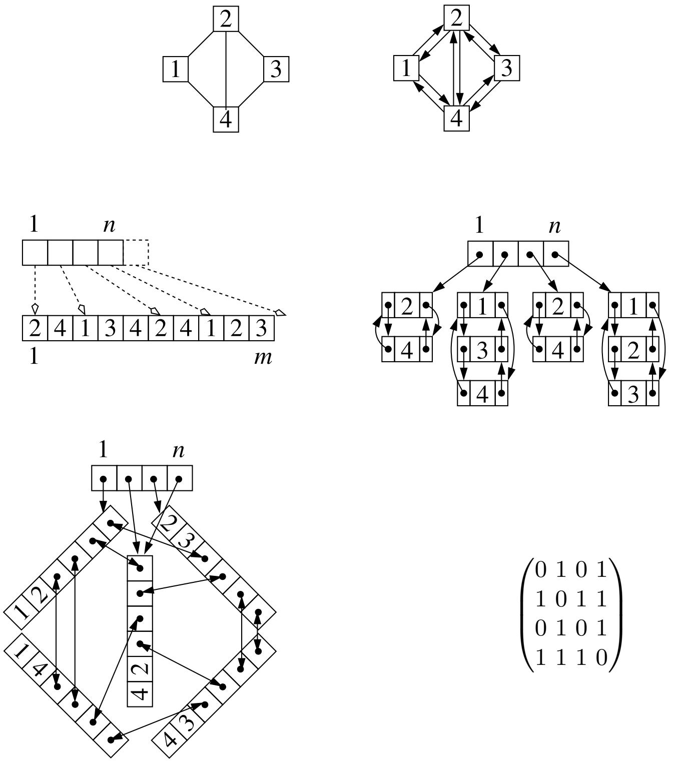


Fig. 8.1. The first row shows an undirected graph and its its interpretation as a bidirected graph. The second row shows the adjacency array and the adjacency list representations of this bidirected graph. The third row shows the linked edge objects representation and the adjacency matrix.

are then easily accessible as $E[V[v]], \ldots, E[V[v+1]-1]$; the dummy entry ensures that this also holds true for node n. Figure 8.1 shows an example.

The memory consumption for storing a directed graph using adjacency arrays is $n + m + \Theta(1)$ words. This is even more compact than the $2m$ words needed for an edge sequence representation.

Adjacency array representations can be generalized to store additional information: we may store information associated with edges in separate arrays or within the edge array. If we also need incoming edges, we may use additional arrays V' and E' to store the reversed graph.

Exercise 149. Design a linear time algorithm for converting an edge sequence representation of a directed graph into an adjacency array representation. You should use only $O(1)$ auxiliary space. Hint: view the problem as the task to sort edges by their source node and adapt the integer-sorting algorithm from Figure 5.15.

8.3 Adjacency Lists — Dynamic Graphs

Edge arrays are a compact and efficient graph representation. Their main disadvantage is that it is expensive to add or remove edges. For example, assume we want to insert a new edge (u, v). Even if there is room in the edge array E to accommodate it, we still have to move the edges associated with nodes $u + 1$ to n one position to the right which takes time $\mathcal{O}(m)$.

In Chapter 3 we learned how to implement dynamic sequences. We can use any of the solutions presented there to arrive at a dynamic graph data structure. For each node v, we represent the sequence E_v of outgoing (or incoming or outgoing and incoming) edges by an an unbounded array or by a (singly or doubly) linked list. We inherit the advantages and disadvantages of the respective sequence representations. Unbounded arrays are more cache efficient. Linked lists allow constant time insertion and deletion of edges at arbitrary positions. Most graphs arising in practice are sparse in the sense that every node has only a few incident edges. Adjacency lists for sparse graphs should be implemented without the header item introduced in Section 3.1 because an additional item would waste considerable space. In the example in Figure 8.1 we show circularly linked lists.

Exercise 150. Suppose the edges adjacent to a node u are stored in an unbounded array E_u and an edge $e = (u, v)$ is specified by giving its position in E_u. Explain how to remove $e = (u, v)$ in constant amortized time. Hint: you do *not* have to maintain the relative order of the other edges.

Exercise 151. Explain how to implement the algorithm for testing whether a graph is acyclic discussed in Chapter 2.9 so that it runs in linear time, i.e., design an appropriate graph representation and an algorithm using it efficiently. Hint: maintain a queue of nodes with outdegree zero.

Bidirected graphs arise frequently. Undirected graphs are naturally presented as bidirected graphs and some algorithms on directed graphs need access not only to outgoing edges but also to incoming edges. In these situations, we frequently want to store the information associated with the undirected edge or the directed edge and its reversal only once. Also, we may want to have easy access from an edge to its reversal.

We will describe two solutions. The first solution simply associates two additional pointers with every directed edge. One points to the reversal and the other points to the information associated with the edge.

The second solution has only one item for each undirected edge (or pair of directed edges) and makes this item a member of two adjacency lists. So the item for undirected edge $\{u, v\}$ would be a member of lists E_u and E_v. If we want doubly linked adjacency information, the edge object for any edge $\{u, v\}$ stores four pointers: two are used for the doubly linked list representing E_u and two are used for the doubly linked list representing E_v. Any node stores a pointer to some edge incident to it. Starting from it, all edges incident to the node can be traversed. The bottom part of Figure 8.1 gives an example. A small complication lies in the fact that finding the other end of an edge now requires some work. Note that the edge object for an edge $\{u, v\}$ stores the endpoints in no particular order. Hence, when we explore the edges out of a node u, we must inspect both endpoints and then choose the one which is different from u. An elegant alternative is to store $u \oplus v$ in the edge object [138]. Then the exclusive-or with either endpoint yields the other endpoint. Also, the representation is more space-efficient.

8.4 Adjacency Matrix Representation

[change notation for vectores and matrices (nonfat?)] An n-node graph can be $\Longleftarrow$ represented by an $n \times n$ *adjacency matrix* $\mathbf{A}$. $\mathbf{A}_{ij}$ is 1 if $(i, j) \in E$ and 0 otherwise. Edge insertion or removal and edge queries work in constant time. It takes time $\mathcal{O}(n)$ to get the edges entering or leaving a node. This is only efficient for very dense graphs with $m = \Omega(n^2)$. Storage requirement is n^2 bits and, for very dense graphs, this may be better than the $n + m + \mathcal{O}(1)$ words required for adjacency arrays. However, even for dense graphs, the advantage is small if additional edge information is needed.

Exercise 152. Explain how to represent an undirected loopless graph with n nodes using $n(n-1)/2$ bits.

Perhaps more important than actually storing the adjacency matrix is the conceptual link between graphs and linear algebra introduced by the adjacency matrix. On the one hand, graph theoretic problems can be solved using methods from linear algebra. For example, if $\mathbf{C} = \mathbf{A}^k$, then $\mathbf{C}_{ij}$ counts the number of paths from i to j with exactly k edges.

Exercise 153. Explain how to store an $n \times n$ matrix $\mathbf{A}$ with m nonzero entries using storage $\mathcal{O}(m + n)$ such that a matrix vector multiplication $\mathbf{Ax}$ can be performed in time $\mathcal{O}(m + n)$. Describe the multiplication algorithm. Expand your representation so that products of the form $\mathbf{x}^T\mathbf{A}$ can also be computed in time $\mathcal{O}(m + n)$.

On the other hand, graph theoretic concepts can be useful for solving problems from linear algebra. For example, suppose we want to solve the matrix equation $\mathbf{Bx} = \mathbf{c}$ where B is a symmetric matrix. Now consider the corresponding adjacency matrix $\mathbf{A}$ where $\mathbf{A}_{ij} = 1$ if and only if $\mathbf{B}_{ij} \neq 0$. If an algorithm for computing connected components finds out that the undirected graph represented by $\mathbf{A}$ contains two disconnected components, this information can be used to reorder the rows and columns of $\mathbf{B}$ such that we get an equivalent equation of the form

$$\begin{pmatrix} \mathbf{B}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{B}_2 \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \end{pmatrix} .$$

This equation can now be solved by solving $\mathbf{B}_1\mathbf{x}_1 = \mathbf{c}_1$ and $\mathbf{B}_2\mathbf{x}_2 = \mathbf{c}_2$ separately. In practice, the situation is more complicated since we rarely get disconnected matrices. Still, more sophisticated graph theoretic concepts such as cuts can help to discover structure in the matrix which can then be exploited in solving problems in linear algebra.

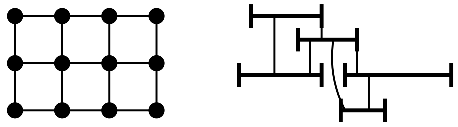


Fig. 8.2. The grid graph G_{34} (left) and an interval graph with 5 nodes and 6 edges (right).

8.5 Implicit Representation

Many applications work with graphs of special structure. Frequently, this structure can be exploited to obtain simpler and more efficient representations. We will give two examples.

The *grid graph* $G_{k\ell}$ with node set $V = [0..k-1] \times [0..\ell-1]$ and edge set

$$E = \left\{((i,j),(i,j')) \in V^2 : |j-j'| = 1\right\} \cup \left\{((i,j),(i',j)) \in V^2 : |i-i'| = 1\right\}$$

is completely defined by the two parameters k and ℓ. Figure 8.2 shows $G_{3,4}$. Edge weights could be stored in two two-dimensional arrays, one for the vertical edges and one for the horizontal edges.

An *interval graph* is defined by a set of intervals. For each interval we have a node in the graph and two nodes are adjacent if the corresponding intervals overlap.
⟹ [removed: An interval graph may be specified by listing its intervals.]

Exercise 154 (Representation of Interval Graphs). (a) Show that for any set of n intervals there is a set of intervals whose endpoints are integers in $[1..2n]$ and that defines the same graph. (b) Devise an algorithm that decides whether the graph defined by a set of n intervals is connected. Hint: sort the endpoints of the intervals and then scan over the endpoints in sorted order. Keep track of the number of intervals that have started but not ended. (c*) Devise a representation for interval graphs that needs $\mathcal{O}(n)$ space and supports efficient navigation. Given an interval I, you need to find all intervals I' intersecting it; I' intersects I if I contains an endpoint of I' or $I \subseteq I'$. How can you find the former and the latter kind of intervals.

8.6 Implementation Notes

We have seen several representations of graphs. They are suitable for different sets of operations on graphs and can be tuned further for maximum performance in a particular application. The edge sequence representation is good only in specialized situations. Adjacency matrices are good for rather dense graphs. Adjacency lists are good if the graph changes frequently. Very often some variant of adjacency arrays is fastest. This may be true even if the graph changes because often there are only few changes or all changes happen in an initialization phase of a graph algorithm, changes can be agglomerated into occasional rebuildings of the graph, or changes can be simulated by building several related graphs.

There are many variants of adjacency array representations. Information associated with nodes and edges may be stored together with these objects or in separate arrays. A rule of thumb is that information that is frequently accessed should be stored with the nodes and edges. Rarely used data should be kept in separate arrays because otherwise it would often be moved to the cache without being used. However, there can be other, more complicated reasons why separate arrays are faster. For example, if both adjacency information and edge weights are read but only the weights are changed then separate arrays may be faster because the amount of data written back to the main memory is reduced.

Unfortunately, no graph representation is best for all purposes. How can one cope with the zoo of graph representations? First, libraries such as LEDA or the Boost graph library offer different graph data types and one of them may suit your purposes. Second, if your application is not particularly time or space critical, several representations might do and there is no need to devise a custom-built representation for the particular application. Third, we recommend to write graph algorithms in the style of generic programming [71]. The algorithms should access the graph data structure only through a small set of operations, such as iterating over the edges out of a node, accessing information associated with an edge, and proceeding to the target node of an edge. The interface can be captured in an interface description and a graph algorithm can be run on any representation realizing the interface. In this way, one can experiment with different representations. [removed:The template mechanism of C++ is a convenient way to encapsulate interfaces.] Fourth, if ⟸ you have to build a custom representation for your application, make it available to others.

C++: [dissolvod long sentence] LEDA [127, 115] offers a very powerful graph ⟸ data type that supports a large variety of operations in constant time, is convenient to use, but space consuming. There LEDA also implements several more space-efficient adjacency array representations.

The Boost graph library [28] emphasizes a strict separation of representation and interface. In particular, Boost graph algorithms run on any representation realizing the Boost interface. Boost also offers its own graph representation class $adjacency\_list$. A large number of parameters allow choosing between variants of graphs (directed, undirected, multigraph), type of available navigation (in-edges, out-edges, ...) and representations of vertex and edge sequences (arrays, linked lists, sorted sequences, ...). However, it should be noted that the array representation uses a separate array for the edges adjacent to each vertex.

Java: JDSL [77] offers rich support for graphs in $jdsl.graph$. It has a clear separation between interfaces, algorithms, and representation. It offers an adjacency list representation of graphs that supports directed and undirected edges.

8.7 Historical Notes and Further Findings

Special classes of graphs may result in additional requirements for their representation. An important example are *planar graphs* — graphs that can be drawn in the plane without crossing edges. Here, the ordering of the edges adjacent to a node should be in counterclockwise order with respect to a planar drawing of the graph. In addition, the graph data structure should efficiently support iterating over the edges along a *face* of the graph, a cycle that does not enclose any other node. LEDA offers representations for planar graphs.

Recall that *bipartite graphs* are special graphs where the node set $V = L \cup R$ can be decomposed into two disjoint subsets L and R so that edges are only between nodes in L and R. All representations discussed here also apply to bipartite graphs. In addition, one may want to store the two sides L and R of the graph.

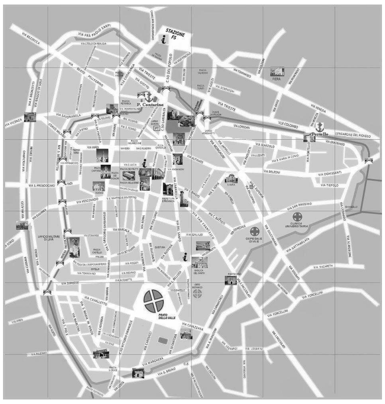
Hypergraphs $H = (V, E)$ are generalizations of graphs where edges can connect more than two nodes. Often hypergraphs are represented as the induced bipartite graph $B_H = (E \cup V, \{(e, v) : e \in E, v \in V, v \in e\})$.

Cayley graphs are an interesting example for implicitly defined graphs. Recall that a set V is a *group* if it has a associative multiplication operation $*$, a neutral element, and a multiplicative inverse operation. The *Cayley graph* (V, E) with respect to a set $S \subseteq V$ has the edge set $\{(u, u * s) : u \in V, s \in S\}$. Cayley graphs are useful because graph theoretic concepts can be useful in group theory. On the other hand, group theory yields concise definitions of many graphs with interesting properties. For example, Cayley graphs have been proposed as the interconnection networks for parallel computers [10].

In this book we have concentrated on convenient data structures for *processing graphs*. There is also a lot of work on *storing* graphs in a flexible, portable, and space efficient way. Significant compression is possible if we have a priori information on the graphs. For example, the edges of a triangulation of n points in the plane can be represented with about $6n$ bits [43, 158].

9

Graph Traversal



Suppose you are working in the traffic planning department of a small town with a nice medieval center. An unholy coalition of shop owners, who want more street-side parking, and the green party, that wants to discourage car traffic all together, have decided to turn most streets into one-way streets. You want to avoid the worst by checking whether the current plan maintains the minimal requirement that one can still drive from every point in town to every other point.

In the language of graphs, see Section 2.9, the question is whether the directed graph formed by the streets is strongly connected. The same problem comes up in other applications. For example, for a communication network with unidirectional channels (e.g., radio transmitters) we want to know who can communicate with whom. Bidirectional communication is possible within the strongly connected components of the graph.

We will present a simple and efficient algorithm for computing strongly connected components (SCCs) in Section 9.2.2. Computing SCCs and many other fundamental problems on graphs can be reduced to systematic graph exploration, inspecting each edge exactly once. We present the two most important exploration strategies: *breadth-first search* in Section 9.1 and *depth-first search* in Section 9.2. Both strategies construct forests and partition the edges into four classes: *tree* edges comprising the forest, *forward* edges running parallel to paths of tree edges, *backward* edges running anti-parallel to paths of tree edges, and *cross* edges that connect two different branches of a tree in the forest. Figure 9.1 illustrates the classification of edges.

9.1 Breadth-First Search

A simple way to explore all nodes reachable from some node s is *breadth-first search (BFS)*. BFS explores the graph *layer* by layer. The starting node s forms layer 0. The

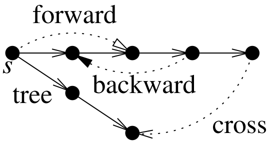


Fig. 9.1. Classification of graph edges into tree edges, forward edges, backward edges, and cross edges.

```
Function bfs($s$ : NodeId) : (NodeArray of NodeId) × (NodeArray of $0..n$)
    $d = \langle\infty,\ldots,\infty\rangle$ : NodeArray of NodeId            // distance from root
    $parent = \langle\bot,\ldots,\bot\rangle$ : NodeArray of NodeId
    $d[s] := 0$
    $parent[s] := s$                                              // self-loop signals root
    $Q = \langle s\rangle$ : Set of NodeId                                  // current layer of BFS-tree
    $Q' = \langle\rangle$ : Set of NodeId                                   // next layer of BFS-tree
    for $\ell := 0$ to $\infty$ while $Q \neq \langle\rangle$ do                        // explore layer by layer
        invariant $Q$ contains all nodes with distance $\ell$ from $s$
        foreach $u \in Q$ do
            foreach $(u,v) \in E$ do                                  // scan edges out of $u$
                if $parent(v) = \bot$ then                        // found an unexplored node
                    $Q' := Q' \cup \{v\}$                              // remember for next layer
                    $d[v] := \ell + 1$
                    $parent(v) := u$                                  // update BFS-tree
        $(Q,Q') := (Q',\langle\rangle)$                                     // switch to next layer
    return $(d, parent)$          // the BFS-tree is now $\{(v,w) : w \in V, v = parent(w)\}$
```

Fig. 9.2. Breadth-first search starting at a node s.

direct neighbors of s form layer 1. In general, all nodes that are neighbors of a node in layer i but not neighbors of nodes in layers $0,\ldots,i-1$ form layer $i+1$.

The algorithm in Figure 9.2 takes a node s and constructs the BFS-tree rooted at s. For each node v in the tree, it records its distance $d(v)$ from s and the parent node $parent(v)$ from which v was first reached. The algorithm returns the pair $(d, parent)$. Initially, s is reached and all other nodes store some special value $\bot$ to indicate that they are not reached yet. Also, the depth of s is zero. The main loop of the algorithm builds the BFS-tree layer by layer. We maintain two sets Q and Q'; Q contains the nodes in the current layer and in Q' we construct the next layer. The inner loops inspect all edges (u,v) leaving nodes u in the current layer Q. Whenever v has no parent pointer yet, we put it into the next layer Q' and set parent pointer and distance appropriately. Figure 9.3 gives an example for a BFS-tree and the resulting backward and cross edges.

BFS has the useful feature that its tree edges define paths from s that have a minimum number of edges. For example, you could use such paths to find railway connections that minimize the number of times you have to change trains or to find paths in communication networks with a minimal number of hops. An actual path from s to a node v can be found by following the parent references from v backwards.

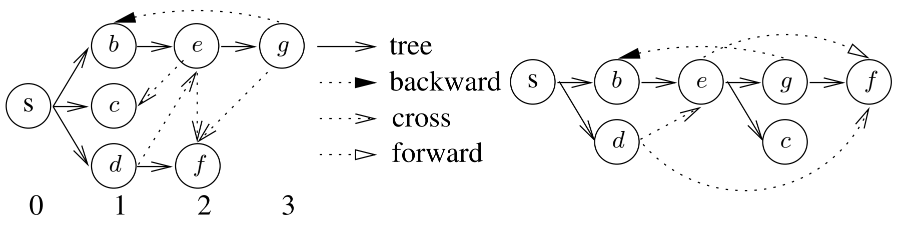


Fig. 9.3. An example how BFS (left) and DFS (right) classify edges into tree edges, backward edges, cross edges and forward edges. BFS visits the nodes in the order s, b, c, d, e, f, g. DFS visits the nodes in the order s, b, e, g, f, c, d.

Exercise 155. Show that BFS will never classify an edge as forward, i.e., there are no edges (u, v) with $d(v) > d(u) + 1$.

Exercise 156. Explain what can go wrong with our implementation of BFS if $\mathit{parent}[s]$ would be initialized to $\perp$ rather than s. Give an example of an erroneous computation.

Exercise 157. BFS-trees are not necessarily unique. In particular, we have not specified in which order nodes are removed from the current layer. Give the BFS-tree that is produced when d is removed before b when doing BFS from node s in the graph from Figure 9.3.

Exercise 158 (FIFO BFS). Explain how to implement BFS using a single FIFO queue of nodes whose outgoing edges still have to be scanned. Prove that the two algorithms compute exactly the same tree if our two-queue algorithm traverses the queues in an appropriate order. Compare the FIFO version of BFS with Dijkstra's algorithm in Section 10.3, and the Jarník-Prim algorithm in Section 11.2. What do they have in common? What are the main differences?

Exercise 159 (Graph representation for BFS). Give a more detailed description of BFS. In particular make explicit how to implement it using the adjacency array representation from Section 8.2. Your algorithm should run in time $\mathcal{O}(n + m)$.

Exercise 160 (Connected components). Explain how to modify BFS so that it computes a spanning forest of an undirected graph in time $\mathcal{O}(m + n)$. In addition, your algorithm should select a *representative* node for each connected component of the graph and assign a value $\mathit{component}[v]$ to each node that identifies this representative. Hint: start BFS from each node $s \in V$ but only reset the parent array once in the beginning. Note that isolated nodes are simply connected components of size one.

Exercise 161 (Transitive closure). The *transitive closure* $G^+ = (V, E^+)$ of a graph $G = (V, E)$ has an edge $(u, v) \in E^+$ whenever there is a path from u to v in E. Design an algorithm for computing transitive closures. Hint: run $\mathit{bfs}(v)$ for each node v to find all nodes reachable from v. Try to avoid the full reinitialization of arrays d and parent at the beginning of each call. What is the running time of your algorithm?

9.2 Depth-First Search

You may view breadth-first search (BFS) as a careful, conservative strategy for systematic exploration that looks at known things before venturing into unexplored territory; in this respect *depth-first search (DFS)* is the exact opposite: whenever it finds a new node, it immediately continues to explore from it. It goes back to previously explored nodes only if it runs out of options. Although DFS leads to unbalanced and strange-looking exploration trees compared to the orderly layers generated by BFS, the combination of eager exploration with the perfect memory of a computer makes DFS very useful. Figure 9.4 gives an algorithm template for DFS. We derive specific algorithms from it by specifying the subroutines init, root, $\mathit{traverseTreeEdge}$, $\mathit{traverseNonTreeEdge}$, and $\mathit{backtrack}$.

DFS marks a node when it first discovers it; initially all nodes are unmarked. The main loop of DFS looks for unmarked nodes s and calls $\mathit{DFS}(s, s)$ to grow a tree rooted at s. The generic call $\mathit{DFS}(u, v)$ explores all edges (v, w) out of v. The argument (u, v) indicates that v was reached via the edge (u, v) into v. For root nodes s, we use the "dummy" argument (s, s). We write $\mathit{DFS}(*, v)$ if the specific nature of the incoming edge is irrelevant for the discussion at hand. Assume now that we explore edge (v, w) within the call $\mathit{DFS}(*, v)$.

If w has been seen before, w is already a node of the DFS-tree. So (v, w) is not a tree edge and hence we call $\mathit{traverseNonTreeEdge}(v, w)$ and make no recursive call of DFS.

If w has not been seen before, (v, w) becomes a tree edge. We therefore call $\mathit{traverseTreeEdge}(v, w)$, mark w and make the recursive call $\mathit{DFS}(v, w)$. When we return from this call we explore the next edge out of v. Once all edges out of v are explored, we call $\mathit{backtrack}$ on the incoming edge (u, v) to perform any summarizing or clean-up operations needed and return.

At any point in time during the execution of DFS, there are a number of active calls. More precisely, there are nodes v_1, v_2, $\ldots v_k$ such that we are currently exploring edges out of v_k, and the active calls are $\mathit{DFS}(v_1, v_1)$, $\mathit{DFS}(v_1, v_2)$, …, $\mathit{DFS}(v_{k-1}, v_k)$. In this situation, we say that the nodes v_1, v_2, …, v_k are *active* and form the DFS recursion stack. Strictly speaking, the recursion stack contains the sequence $\langle (v_1, v_1), (v_1, v_2), \ldots, (v_{k-1}, v_k) \rangle$, but we prefer the more concise formulation. The node v_k is called the *current node*. We say that a node v is reached, when $\mathit{DFS}(*, v)$ is called, and is finished, when the call $\mathit{DFS}(*, v)$ terminates.

Exercise 162. Give a non-recursive formulation of DFS. You need to maintain a stack of active nodes and for each active node the set of unexplored edges.

9.2.1 DFS Numbering, Finishing Times, and Topological Sorting

DFS has numerous applications. In this section, we use it to number the nodes in two ways. As a byproduct, we see how to decide acyclicity of graphs. We number the nodes in the order in which they are reached (array dfsNum) and in the order in which they are finished (array $\mathit{finishTime}$). We have two counters dfsPos

```
Depth-first search of a directed graph $G = (V, E)$
unmark all nodes
init
foreach $s \in V$ do
    if $s$ is not marked then
        mark $s$                                    // make $s$ a root and grow
        root$(s)$                                   // a new DFS-tree rooted at it.
        DFS$(s, s)$

Procedure DFS$(u, v : NodeId)$                      // Explore $v$ coming from $u$.
    foreach $(v, w) \in E$ do
        if $w$ is marked then traverseNonTreeEdge$(v, w)$    // $w$ was reached before
        else    traverseTreeEdge$(v, w)$                      // $w$ was not reached before
                mark $w$
                DFS$(v, w)$
    backtrack$(u, v)$                               // return from $v$ along the incoming edge
```

Fig. 9.4. A template for depth-first search of a graph $G = (V, E)$. We say that a call $DFS(*, v)$ explores v. The exploration is complete when we return from this call.

and *finishingTime*, both initialized to one. When we encounter a new root or traverse a tree edge, we set *dfsNum* of the newly encountered node and increment *dfsPos*. When we backtrack from a node, we set its *finishTime* and increment *finishingTime*. We use the following subroutines:

$init$:	$dfsPos = 1 \ : 1..n$; $\ finishingTime = 1 \ : 1..n$
$root(s)$:	$dfsNum[s] := dfsPos{+}{+}$
$traverseTreeEdge(v, w)$:	$dfsNum[w] := dfsPos{+}{+}$
$backtrack(u, v)$:	$finishTime[v] := finishingTime{+}{+}$

The ordering by *dfsNum* is so useful that we introduce a special notation "$\prec$" for it. For any two nodes u and v, we define

$$u \prec v \Leftrightarrow dfsNum[u] < dfsNum[v] \ .$$

The numberings *dfsNum* and *finishTime* encode important information about the execution of *DFS* as we will show next. We will first show that DFS-numbers increase along any path of the DFS-tree and then show that the numbering together classify the edges according to their types.

Lemma 21. *The nodes on the DFS recursion stack are sorted with respect to* $\prec$.

Proof. *dfsPos* is incremented after every assignment to *dfsNum*. Thus, when a node v becomes active by a call $DFS(u, v)$, it has just been assigned the largest *dfsNum* so far.

*dfsNum*s and *finishTime*s classify edges according to their types as shown in Figure 9.5. The argument is as follows. Two calls of DFS are either nested

type	$\mathit{dfsNum}[v] < \mathit{dfsNum}[w]$	$\mathit{finishTime}[w] < \mathit{FinishTime}[v]$
tree	yes	yes
forward	yes	yes
backward	no	no
cross	yes	no

Fig. 9.5. The classification of an edge (v, w). Tree and forward edges are also easily distinguished. Tree edges lead to recursive calls and forward edges do not.

within each other, i.e., when the second call starts the first is still active, or disjoint, i.e., when the second starts the first is already completed. If $DFS(*, w)$ is nested in $DFS(*, v)$ the former call starts after the latter and finishes before it, i.e., $\mathit{dfsNum}[v] < \mathit{dfsNum}[w]$ and $\mathit{finishTime}[w] < \mathit{finishTime}[v]$. If $DFS(*, w)$ and $DFS(*, v)$ are disjoint and the former call starts before the latter it also ends before the latter, i.e., $\mathit{dfsNum}[w] < \mathit{dfsNum}[v]$ and $\mathit{finishTime}[w] < \mathit{finishTime}[v]$. The tree edges record the nesting structure of recursive calls. When a tree edge (v, w) is explored within $DFS(*, v)$, the call $DFS(v, w)$ is made and hence nested within $DFS(*, v)$. Thus w has a larger DFS-number and a smaller finishing time than v. A forward edge (v, w) runs parallel to a path of tree edges and hence w has a larger DFS-number and a smaller finishing time than v. A backward edge (v, w) runs anti-parallel to a path of tree edges and hence w has a smaller DFS-number and a larger finishing time than v. Let us finally look at a cross-edge (v, w). Since (v, w) is not a tree, forward, or backward edge, the calls $DFS(*, v)$ and $DFS(*, w)$ cannot be nested within each other. Thus they are disjoint. So w is either marked before $DFS(*, v)$ starts or after it ends. The latter case is impossible, since, in this case, w would be unmarked when the edge (v, w) is explored and the edge would become a tree edge. So w is marked before $DFS(*, v)$ starts and hence $DFS(*, w)$ starts and ends before $DFS(*, v)$. Thus $\mathit{dfsNum}[w] < \mathit{dfsNum}[v]$ and $\mathit{finishTime}[w] < \mathit{finishTime}[v]$. We summarize the discussion in

Lemma 22. *Figure 9.5 shows the characterization of edge types in terms of dfsNum and finishTime.*

Exercise 163. Modify DFS such that it labels the edges with their type. What is the type of an edge (v, w) when w is on the recursion stack when the edge is explored?

Finishing times have an interesting property for directed acyclic graphs.

Lemma 23. *The following properties are equivalent: (i) G is an acyclic directed graph (DAG). (ii) DFS on G produces no backward edge. (iii) All edges of G go from larger to smaller finishing times.*

Proof. Backward edges run anti-parallel to paths of tree edges and hence create cycles. Thus DFS of an acyclic graph cannot create any backward edge. All other types of edges run from larger to smaller finishing time according to Figure 9.5. Assume next that all edges run from larger to smaller finishing time. Then the graph is clearly acyclic.

An order of the nodes of a DAG in which all edges go from left to right[was:earlier to later nodes] is called a *topological sorting*. By Lemma 23, the ordering by decreasing finishing time is a topological ordering. Many problems on DAGs can be solved efficiently by iterating over the nodes in topological order. For example, in Section 10.2 we will see a fast and simple algorithm for computing shortest paths in acyclic graphs. ⟸

Exercise 164 (Topological sorting). Design a DFS-based algorithm that outputs the nodes in topological order if G is a DAG. Otherwise it should output a cycle.

Exercise 165. Design a BFS-based algorithm for topological sorting.

Exercise 166. Show that DFS on an undirected graph does not produce any cross edges.

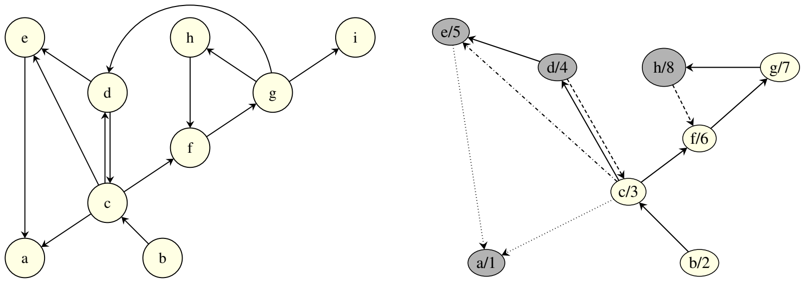
9.2.2 *Strongly connected components (SCCs)

We now come back to the problem posed at the beginning of this chapter. Recall that two nodes belong to the same strongly connected component (SCC) of a graph iff they are reachable from each other. In undirected graphs, the relation "being reachable" is symmetric and hence strongly connected components are the same as connected components. Exercise 160 outlines how to compute connected components using BFS and adapting this idea to DFS is equally simple. In directed graphs the situation is more interesting, see Figure 9.6 for an example. We show that an extension of DFS computes the strongly connected components of a directed graph G in linear time $\mathcal{O}(n + m)$. More precisely, the algorithm will output an array *component* indexed by nodes such that $component[v] = component[w]$ iff v and w belong to the same SCC. Alternatively, it could output the node set of each SCC.

[probleme mit 9.6: Die beiden Graphen sollten gleich gezeichnet sein. Kanten sollten so klassifziert werden wie vorher. Beschriftung grÃűÃ§er und mit math fonts. letzten Satz der caption gestrichen] ⟸

Consider a depth-first search on G and use $G_c = (V_c, E_c)$ to denote the subgraph already explored, i.e., V_c comprises the marked nodes and E_c comprises the explored edges. The algorithm maintains the strongly connected components of G_c. In order to derive the algorithm, we first introduce some notation and then state some properties of G_c. We call an SCC *open* if it contains an unfinished node and *closed* otherwise. We call a node open if it belongs to an open component and closed if it belongs to a closed component. Observe that a closed node is always finished and an open node may be finished or unfinished. In every component, we single out one node, namely the node with the smallest DFS-number in the component, and call it the representative of the component. Figure 9.6 illustrates these concepts. The following statements capture important properties of G_c; see also Figure 9.7.

(1) All edges in G (not just G_c) out of closed nodes lead to closed nodes. In our example, the nodes a and e are closed.



open nodes	b	c	d	f	g	h
representatives	b	c		f		

Fig. 9.6. The graph on the left has five strongly connected components, namely the subgraphs spanned by the node sets $\{a\}$, $\{b\}$, $\{e\}$, $\{c, d, f, g, h\}$, and $\{i\}$. The picture on the right shows a snapshot of depth-first search on this graph. A first DFS was started at node a and a second DFS was started at node b, the current node is g and the recursion stack contains b, c, f, g. The depth-first search numbers of the nodes are indicated. The edges (g, i) and (g, d) have not been explored yet. Completed nodes are shaded. In G_c there are the closed components $\{a\}$ and $\{e\}$ and open components $\{b\}$, $\{c, d\}$, and $\{f, g, h\}$. The representatives of the open components are the nodes b, c, and f, respectively.

(2) The tree path to the current node contains the representatives of all open components. Let S_1 to S_k be the open components as they are traversed by the tree path to the current node. Then there is a tree edge from a node in S_{i-1} to the representative of S_i and this is the only edge into S_i, $2 \leq i \leq k$. Also, there is no edge from a S_j to a S_i with $i < j$. Finally, all nodes in S_j are reachable from the representative r_i of S_i for $1 \leq i \leq j \leq k$. In our example, the current node is g. The tree path $\langle b, c, f, g\rangle$ to the current node contains the open representatives b, c, and f. Every open component forms a subtree of the depth-first search tree.

(3) Consider the nodes in open components ordered by their DFS-numbers. The representatives partition the sequence into the open components. In our example, the sequence of open nodes is $\langle b, c, d, f, g, h\rangle$ and the representatives partition this sequence into the open components $\{b\}$, $\{c, d\}$, and $\{f, g, h\}$.

We will show below that all three properties hold true generally and not only for our example. The four properties will be invariants of the algorithm to be developed. The first invariant implies that the closed SCCs of G_c are actually SCCs of G, i.e., it is justified to call them closed. This observation is so important that it deserves to be stated as a lemma.

Lemma 24. *A closed SCC of G_c is an SCC of G.*

Proof. Let v be a closed vertex, let S be the SCC of G containing v, and let S_c be the SCC of G_c containing v. We need to show that $S = S_c$. Since G_c is a subgraph of G, we have $S_c \subseteq S$. So, it suffices to show $S \subseteq S_c$. Let w be any vertex in S.

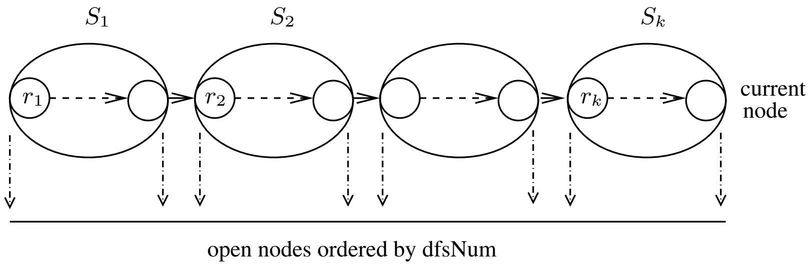


Fig. 9.7. The open SCCs are indicated as ovals and the current node is shown as a circle. The tree path to the current node is indicated. It enters each component at its representative. The horizontal line below represents the open nodes ordered by $dfsNum$. Each open SCC forms a contiguous subsequence with its representative as its leftmost element.

Then there is a cycle in G passing through v and w. The first invariant implies that all vertices of C are closed. Since closed vertices are finished, all edges out of them have been explored. Thus C is contained in G_c and hence $w \in S_c$.

Invariants (2) and (3) suggest a simple method to represent the open SCCs of G_c. We simply keep a sequence $oNodes$ of all open nodes in increasing order of DFS-numbers and the subsequence $oReps$ of open representatives. In our example, we have $oNodes = \langle b, c, d, f, g, h \rangle$ and $oReps = \langle b, c, f \rangle$. We will later see that the type $stack$ **of** $nodeId$ is appropriate for both sequences.

Let us next see how the SCCs of G_c develop during DFS. We discuss the various actions of DFS one by one and show that the invariants are maintained. We also discuss how to update our representation of the open components.

When DFS starts, the invariants clearly hold: no node is marked, no edge has been traversed, G_c is empty, and hence there are neither open nor closed components yet. Our sequences $oNodes$ and $oReps$ are empty.

Before a new root is marked, all marked nodes are finished and hence there can only be closed components. Therefore, both sequences $oNodes$ and $oReps$ are empty and marking a new root s produces the open component $\{s\}$. The invariants are clearly maintained. We obtain the correct representation by adding s to both sequences.

If a tree edge $e = (v, w)$ is traversed and hence w becomes marked, $\{w\}$ becomes an open component of its own. All other open components are unchanged. The first invariant is clearly maintained, since v is active and hence open. The old current node is v and the new current node is w. The sequence of open components is extended by $\{w\}$. The open representatives are the old open representatives plus the node w. Thus the second invariant is maintained. Also, w becomes the open node with the largest DFS-number and hence $oNodes$ and $oReps$ are both extended by w. Thus the third invariant is maintained.

Now suppose a non-tree edge $e = (v, w)$ out of the current node v is explored. If w is closed, the SCCs of G_c do not change by adding e to G_c since by Lemma 24 the SCC of G_c containing w is already an SCC of G *before* e is traversed. So assume

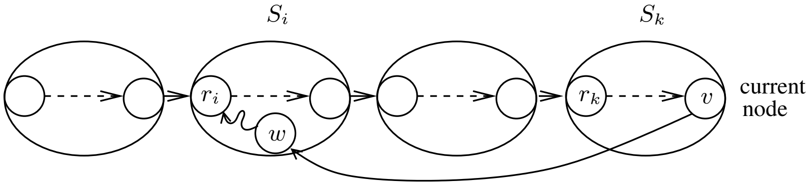


Fig. 9.8. The open SCCs are indicated as ovals and their representatives as circles. All representatives lie on the tree path to the current node v. The non-tree edge $e = (v, w)$ ends in an open SCC S_i with representative r_i. There is a path from w to r_i since w belongs to the SCC with representative r_i. Thus the edge (v, w) merges S_i to S_k into a single SCC.

that w is open. Then w lies in some open SCC S_i of G_c. We claim that the SCCs S_i to S_k are merged into a single component and all other components are unchanged. Indeed, let r_i be the representative of S_i. Then we can go from r_i to v along a tree path by invariant (2), then follow the edge (v, w), and finally return to r_i. The path from w to r_i exists since w and r_i lie in the same SCC of G_c. We conclude that any node in an S_j with $i \leq j \leq k$ can be reached from r_i and can reach r_i. Thus the SCCs S_i to S_k become one SCC and r_i is their representative. The S_j with $j < i$ are unaffected by addition of the edge.

The third invariant tells us how to find r_i, the representative of the component containing w. The sequence $oNodes$ is ordered by $dfsNum$ and the representative of an SCC has the smallest $dfsNum$ of any node in the component. Thus $dfsNum[r_i] \leq dfsNum[w]$ and $dfsNum[w] < dfsNum[r_j]$ for all $j > i$. It is therefore easy to update our representation. We simply delete all representatives r with $dfsNum[r] > dfsNum[w]$ from $oReps$.

Finally, we need to consider finishing a node v. When will this close an SCC? By invariant (2), all nodes in a component are tree descendants of the representative of the component and hence the representative of a component is the last node to finish in the component. In other words, we close a component iff we finish a representative. Since $oReps$ is ordered by $dfsNum$ we close a component iff the last node of $oReps$ finishes. So assume, we finish a representative v. Then by invariant (3), the component S_k with representative $v = r_k$ consists of v and all nodes in $oNodes$ following v. Finishing v closes S_k. By invariant (2) there is no edge out of S_k into an open component. Thus invariant (1) holds after closing S_k. The new current node is the parent of v. By invariant (2), the parent of v lies in S_{k-1}. Thus invariant (2) holds after closing S_k. Invariant (3) holds after removing v from $oReps$ and v and all nodes following it from $oNodes$.

It is now easy to instantiate the DFS template. Figure 9.10 shows the pseudocode and Figure 9.9 illustrates a complete run. We use an array $component$ indexed by nodes to record the result and two stacks $oReps$ and $oNodes$. When a new root is marked or a tree edge is explored, a new open component consisting of a single node is created by pushing this node onto both stacks. When a cycle of open components is created, these components are merged by popping representatives from $oReps$ as long as the top representative is not to the left of the node w closing the cycle. An

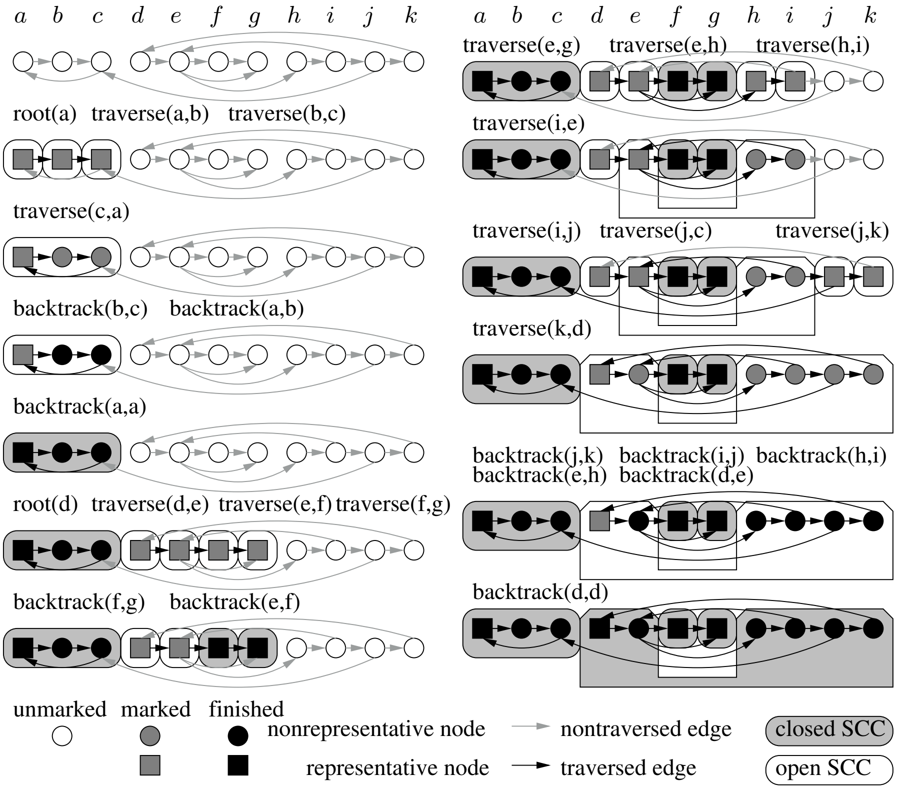

a b c d e f g h i j k
root(a) traverse(a,b) traverse(b,c)
traverse(c,a)
backtrack(b,c) backtrack(a,b)
backtrack(a,a)
root(d) traverse(d,e) traverse(e,f) traverse(f,g)
backtrack(f,g) backtrack(e,f)
a b c d e f g h i j k
traverse(e,g) traverse(e,h) traverse(h,i)
traverse(i,e)
traverse(i,j) traverse(j,c) traverse(j,k)
traverse(k,d)
backtrack(j,k) backtrack(i,j) backtrack(h,i)
backtrack(e,h) backtrack(d,e)
backtrack(d,d)
unmarked
marked
finished
nonrepresentative node
representative node
nontraversed edge
traversed edge
closed SCC
open SCC

Fig. 9.9. An example for the development of open and closed SCCs during DFS. Unmarked nodes are shown as empty circles, marked nodes are shown in gray and finished nodes are shown in black. Non-traversed edges are shown in gray and traversed edges are shown in black. Open SCCs are shown as empty ovals and closed SCCs are shown as gray ovals. We start in the situation at the upper left side. We make a a root and traverse the edges (a, b) and (b, c). This creates three open SSCs. The traversal of edge (c, a) merges these components into one. Next we backtrack to b, then to a, and finally from a. At this point, the component becomes closed. Please, complete the description.

SCC S is closed when its representative v finishes. At that point, all nodes of S are stored above v in $oNodes$. Operation $backtrack$ therefore closes S by popping v from $oReps$ and by popping the nodes $w \in S$ from $oNodes$ and setting their $component$ to the representative v.

Note that the test $w \in oNodes$ in $traverseNonTreeEdge$ can be done in constant time by storing information with each node that indicates whether the node is open or not. This indicator is set when a node v is first marked and reset when the component of v is closed. We give implementation details in Section 9.3. Furthermore, the while loop and the repeat loop can make at most n iterations during the entire execution

```
init:
    component : NodeArray of NodeId                       // SCC representatives
    oReps = ⟨⟩ : Stack of NodeId                          // representatives of open SCCs
    oNodes = ⟨⟩ : Stack of NodeId                         // all nodes in open SCCs

root($w$) or traverseTreeEdge($v, w$):
    $oReps.push(w)$                                       // new open
    $oNodes.push(w)$                                      // component

traverseNonTreeEdge($v, w$):
    if $w \in oNodes$ then
        while $w \preceq oReps.top$ do $oReps.pop$        // collapse components on cycle

backtrack($u, v$):
    if $v = oReps.top$ then
        oReps.pop                                         // close
        repeat                                            // component
            $w := oNodes.pop$
            component[$w$] $:= v$
        until $w = v$
```

Fig. 9.10. An instantiation of the DFS template that computes strongly connected components of a graph $G = (V, E)$.

of the algorithm since each node is pushed on the stacks exactly once. Hence, the execution time of the algorithm is $\mathcal{O}(m + n)$. We have the following theorem:

Theorem 26. *The algorithm in Figure 9.10 computes strongly connected components in time $\mathcal{O}(m + n)$.*

Exercise 167 (Certificates). Let G be a strongly connected graph and let s be a node of G. Show how to construct two trees rooted at s. The first tree proves that all nodes can be reached from s and the second tree proves than s can be reached from all nodes.

Exercise 168 (2-edge connected components). Two nodes of an *undirected* graph are in the same 2-edge connected component (2ECC) iff they lie on a common cycle, see Figure 9.11. Show that the SCC algorithm from Figure 9.10 computes 2-edge connected components. Hint: show first that DFS of an undirected graph never produces any cross edges.

Exercise 169 (biconnected components). Two nodes of an *undirected* graph belong to the same *biconnected component (BCC)* iff they are connected by an edge or there are two edge disjoint paths connecting them, see Figure 9.11. A node is an articulation point if it belongs to more than BCC. Design an algorithm that computes biconnected components using a single pass of DFS. Hint: adapt the strongly connected components algorithm. Define the representative of a BCC as the node with

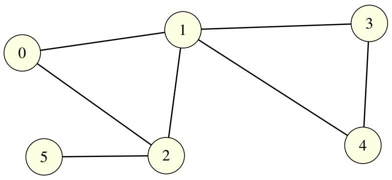


Fig. 9.11. The graph has two 2-edge connected components, namely $\{0, 1, 2, 3, 4\}$ and $\{5\}$. The graph has three biconnected components, namely the subgraphs spanned by the sets $\{0, 1, 2\}$, $\{1, 3, 4\}$ and $\{2, 5\}$. The vertices 1 and 2 are articulation points.

the second smallest $dfsNum$ in the BCC. Prove that a BCC consists of the parent of the representative and all tree descendants of the representative that can be reached without passing through another representative. Modify $backtrack$. When you return from a representative v, output v, all nodes above v in $oNodes$, and the parent of v.

9.3 Implementation Notes

BFS is usually implemented by keeping unexplored nodes (with depths d and $d + 1$) in a FIFO queue. We choose a formulation using two separate sets for nodes at depth d and nodes at depth $d+1$ mainly because it allows a simple loop invariant that makes correctness immediately evident. However, our formulation might also turn out to be somewhat more efficient. If Q and Q' are organized as stacks, we will get less cache faults than for a queue in particular if the nodes of a layer do not quite fit into the cache. Memory management becomes very simple and efficient by allocating just a single array a of n nodes for both stacks Q and Q'. One stack grows from $a[1]$ to the right and the other grows from $a[n]$ to the left. When switching to the next layer, the two memory areas switch their roles.

Our SCC algorithm needs to store four kinds of information for each node v: an indication whether v is marked, an indication whether v is open, something like a DFS-number in order to implement '$\prec$', and, for closed nodes, the $NodeId$ of the representative of its component. The array $component$ suffices to keep this information. For example, if $NodeId$s are integers in $1..n$, $component[v] = 0$ could indicate an unmarked node. Negative numbers can indicate negated DFS-numbers so that $u \prec v$ iff $component[u] > component[v]$. This works because '$\prec$' is never applied to closed nodes. Finally, the test $w \in oNodes$ simply becomes $component[v] < 0$. [more tricks from the scc paper:]With these simplifications in place, additional ⟸ tuning is possible. We make $oReps$ store $component$ numbers of representatives rather than their IDs and save an access to $component[oReps.top]$. Finally, the array $component$ should be stored with the node data as a single array of records.

C++: LEDA has implementations for topological sorting, reachability from a node (DFS), DFS-numbering, BFS, strongly connected components, biconnected components, and transitive closure. BFS, DFS, topological sorting, and strongly connected components are also available in a very flexible implementation ($GIT\_\ldots$) that separates representation and implementation, supports incremental execution, and allows various other adaptations.

The Boost graph library [28] uses the *visitor concept* to support graph traversal. A visitor class has user-definable methods that are called at *event points* during the execution of a graph traversal algorithm. For example, the DFS visitor defines event points similar (there are more event points in Boost) to the operations $init$, $root$, $traverse\ldots$, and $backtrack$ used in our DFS template.

Java: The JDSL library [77] supports DFS in a very flexible way not very much different from the visitor concept described for Boost. There are also more specialized algorithms for topological sorting and finding cycles.

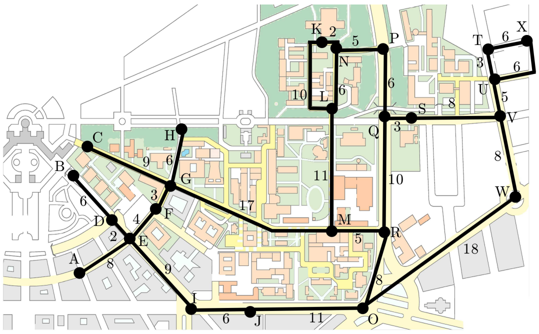
9.4 Historical Notes and Further Findings

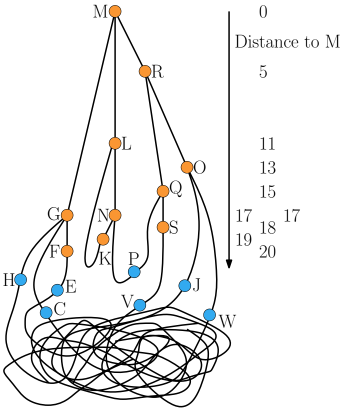
BFS and DFS were known before the age of computers. Tarjan [177] discovered the power of DFS and provided linear time algorithms for many basic problems in graphs, in particular biconnected and strongly connected components. [added some ⟹ more scc refs from paper] Our SCC algorithm was invented by Cheriyan and Mehlhorn [40] and later rediscovered by Gabow [70]. Yet another linear time SCC algorithm is due to Kosaraju and Sharir [167]. It is very simple, yet needs two passes of DFS. DFS can be used to solve many other graph problems in linear time, e.g., ear decomposition, planarity test, planar embeddings, and triconnected components.

It may seem that problems solvable by graph traversal are so simple that little further research is needed for them. However, the bad news is that graph traversal itself is very difficult on advanced models of computations. In particular, DFS is a nightmare for both parallel processing [151] and for memory hierarchies [134, 124]. Therefore alternative ways to solve seemingly simple problems are an interesting area of research. For example, in Section 11.9 we describe an approach to construct minimum spanning trees using *edge contraction* that also works for finding connected components. Furthermore, the problem of finding biconnected components can be reduced to finding connected components [179]. DFS-based algorithms for biconnected components and strongly connected components are almost identical. But this analogy completely disappears for advanced models of computations so that algorithms for strongly connected components remain an area of intensive (and sometimes frustrating) research. More generally, it seems that problems for undirected graphs (such as biconnected components) are often easier to solve than analogous problems for directed graphs (such as strongly connected components).

10

Shortest Paths





The shortest, quickest or cheapest path problem is ubiquitous. You solve it daily. When you are in location s and want to move to location t, you ask for the quickest path from s to t. The fire department may want to compute the quickest routes from a fire station s to all locations in town — the single-source problem. Sometimes, we may even want a complete distance table from everywhere to everywhere — the all-pairs problem. In a road atlas, you usually find an all-pairs distance table for the most important cities.

Here is a route planning algorithm that requires a city map and a lot of dexterity but no computer: lay thin threads along the roads of the city map. Make a knot wherever roads meet and at your starting position. Now lift the starting knot until the entire net dangles below it. If you have successfully avoided any tangles and the threads and your knots are thin enough so that only gravity and tight threads hinder a knot from moving down, the tight threads define shortest paths.

The introductory figure shows the campus map of the University of Karlsruhe and illustrates the route planning algorithm for source node 5.

Route planning in road networks is one of the many applications of shortest path computations. By defining an appropriate graph model, many problems turn out to profit from shortest path computations. For example, Ahuja et al. [8] mention such diverse applications as planning flows in networks, urban housing, inventory planning, DNA sequencing, the knapsack problem (see also Chapter 12), production planning, telephone operator scheduling, vehicle fleet planning, approximating piecewise linear functions, or allocating inspection effort on a production line.

The most general formulation of the shortest path problem looks at a directed graph $G = (V, E)$ and a cost function c that maps edges to arbitrary real number costs. It turns out that the most general problem is fairly expensive to solve. So we are also interested in various restrictions that allow simpler and more efficient algorithms: non-negative edge costs, integer edge costs, or acyclic graphs. Note that

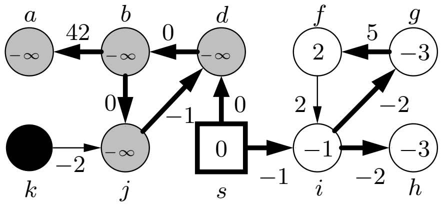


Fig. 10.1. A graph with shortest path distances $\mu(s, v)$. Edge costs are shown as edge labels and the distances are shown inside the nodes. Heavy edges indicate shortest paths.

we have already solved the very special case of unit edge costs in Section 9.1 — the breadth-first search (BFS) tree rooted at node s is a concise representation of all shortest paths from s. We begin in Section 10.1 with basic concepts that lead to a generic approach to shortest path algorithms. The systematic approach will help us to keep track of the zoo of shortest path algorithms. As a first example for a restricted yet fast and simple algorithm we look at acyclic graphs in Section 10.2. In Section 10.3 we come to the most widely used algorithm for shortest paths: Dijkstra's algorithm for general graphs with non-negative edge costs. The efficiency of Dijkstra's algorithm heavily relies on efficient priority queues. In Section 10.4 we discuss *monotone priority queues for integer keys*. Section 10.5 deals with arbitrary edge costs and Section 10.6 treats the all-pairs problem. We show that the all-pairs problem for general edge costs reduces to one general single-source problem plus n single-source problems with non-negative edge costs. The reduction introduces the generally useful concept of node potentials.

10.1 From Basic Concepts to a Generic Algorithm

We extend the cost function to paths in the natural way. The cost of a path is the sum of the costs of its constituent edges, i.e., if $p = \langle e_1, e_2, \ldots, e_k \rangle$ then $c(p) = \sum_{1 \leq i \leq k} c(e_i)$. The empty path has cost zero.

For a pair s and v of nodes, we are interested in a shortest path from s to v. We avoid the use of the definite article "the", since there may be more than one shortest path. Does a shortest path always exist? Observe that the number of paths from s to v may be infinite. For example, if $r = pCq$ is a path from s to v containing a cycle C, then we may go around the cycle an arbitrary number of times and still have a path from s to v, see Figure 10.2. More precisely, p is a path leading from s to u, C is a path leading from u to u and q is a path from u to v. Consider the path $r^{(i)}$ which first uses p to go from s to u, then goes around the cycle i times, and finally follows q from u to v. The cost of $r^{(i)}$ is $c(p) + i \cdot c(C) + c(q)$. If C is a so-called *negative cycle*, i.e., $c(C) < 0$ then $c(r^{(i+1)}) < c(r^{(i)})$. In this situation there is no shortest path from s to v. Assume otherwise, say P is a shortest path from s to v.

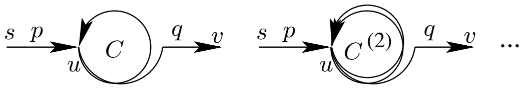


Fig. 10.2. A non-simple path pCq from s to v.

Then $c(r^{(i)}) < c(P)$ for i large enough[1] and so P is not a shortest path from s to v. We will next show that shortest paths exist if there are no negative cycles.

Lemma 25. *If G contains no negative cycle and v is reachable from s then a shortest path from s to v exists. Moreover, the shortest path is simple.*

Proof. Assume otherwise. Let ℓ be the minimal cost of a *simple* path from s to v and assume that there is a non-simple path r from s to v of cost less than ℓ. Since r is non-simple we can, as in Figure 10.2, write r as pCq, where C is a cycle and pq is a simple path. Then $\ell \leq c(pq)$ and hence $c(pq) + c(C) = c(r) < \ell \leq c(pq)$. So $c(C) < 0$ and we have shown the existence of a negative cycle.

Exercise 170. Strengthen the lemma above and show: if v is reachable from s then a shortest path from s to v exists iff there is no negative cycle that is reachable from s and from which one can reach v.

For two nodes s and v, we define the shortest path distance $\mu(s, v)$ from s to v as

$$\mu(s,v) := \begin{cases} +\infty & \text{if there is no path from } s \text{ to } v \\ -\infty & \text{if there is no shortest path from } s \text{ to } v \\ c(\text{a shortest path from } s \text{ to } v) & \text{otherwise.} \end{cases}$$

Observe that if v is reachable from s, but there is no shortest path from s to v, then there are paths of arbitrarily large negative cost. Thus it makes sense to define $\mu(s, v) = -\infty$ in this case. Shortest paths have further nice properties which we state as exercises:

Exercise 171 (Subpaths of Shortest Paths.). Show that subpaths of shortest paths are themselves shortest paths, i.e., if a path of the form pqr is a shortest path than q is also a shortest path.

Exercise 172 (Shortest Path Trees.). Assume that all nodes are reachable from s and that there are no negative cycles. Show that there is an n-node tree T rooted as s such that all tree paths are shortest paths. Hint: assume first that shortest paths are unique and consider the subgraph T consisting of all shortest paths starting at s. Use the preceding exercise to prove that T is a tree. Extend to the case when shortest paths are not unique.

[1] $i > (c(p) + c(q) - c(P))/|c(C)|$ will do.

Our strategy for finding shortest paths from a source node s is a generalization of the BFS algorithm in Figure 9.3. We maintain two $\mathit{NodeArray}$s d and parent. Here $d[v]$ contains our current knowledge about the distance from s to v and $\mathit{parent}[v]$ stores the predecessor of v on the currently shortest path to v. We usually refer to $d[v]$ as the *tentative distance* of v. Initially, $d[s] = 0$ and $\mathit{parent}[s] = s$. All other nodes have infinite distance and no parent.

The natural way to improve distance values is to propagate distance information across edges. If there is a path from s to u of cost $d[u]$ and $e = (u, v)$ is an edge out of u, then there is a path from s to v of cost $d[u] + c(e)$. If this cost is smaller than the best previously known distance $d[v]$, we update d and parent accordingly. This process is called *edge relaxation*.

```
Procedure relax($e = (u, v)$ : Edge)
    if $d[u] + c(e) < d[v]$ then $d[v] := d[u] + c(e)$;    $parent[v] := u$
```

Lemma 26. *After any sequence of edge relaxations: If $d[v] < \infty$, then there is a path of length $d[v]$ from s to v.*

Proof. We use induction on the number of edge relaxations. The claim is certainly true before the first relaxation. The empty path is a path of length zero from s to v and all other nodes have infinite distance. Consider next a relaxation of edge $e = (u, v)$. By induction hypothesis, there is a path p of length $d[u]$ from s to u and a path q of length $d[v]$ from s to v. If $d[u] + c(e) \geq d[v]$, there is nothing to show. Otherwise, pe is a path of length $d[u] + c(e)$ from s to v.

The common strategy of the algorithms in this chapter is to relax edges until either all shortest paths are found or a negative cycle is discovered. For example, the fat edges in Figure 10.1 give us the parent information obtained after a sufficient number of edge relaxations: nodes f, g, i, and h are reachable from s using these edges and have reached their respective $\mu(s, \cdot)$ values 2, -3, -1, and -3. Node b, j, and d form a negative cost cycle so that their shortest path cost is $-\infty$. Node a is attached to this cycle and thus $\mu(s, a) = -\infty$.

What is a good sequence of edge relaxations? Let $p = \langle e_1, \ldots, e_k \rangle$ be a path from s to v. If we relax the edges in the order e_1 to e_k, we have $d[v] \leq c(p)$ after the sequence of relaxations. If p is a shortest path from s to v, then $d[v]$ cannot drop below $c(p)$ by the preceding Lemma and hence $d[v] = c(p)$ after the sequence of relaxations.

Lemma 27 (Correctness Criterion). *After performing a sequence R of edge relaxations, we have $d[v] = \mu(s, v)$ if for some shortest path $p = \langle e_1, e_2, \ldots, e_k \rangle$ from s to v, p is a subsequence of R, i.e., there are indices $t_1 < t_2 < \cdots < t_k$ such that $R[t_1] = e_1, R[t_2] = e_2, \ldots, R[t_k] = e_k$. Moreover, the parent information defines a path of length $\mu(s, v)$ from s to v.*

Proof. Here is a schematic view of R and p: the first row indicates time. At time t_1, the edge e_1 is relaxed, at time t_2, the edge e_2 is relaxed, and so on.

$$\begin{array}{rcccccccc} & 1,2,\ldots, & t_1, & \ldots, & t_2, & \ldots\ldots & ,t_k, & \ldots & \\ R := \langle & \ldots & ,e_1, & \ldots, & e_2, & \ldots\ldots & ,e_k, & \ldots\rangle & \\ p{:=} & & \langle e_1, & & e_2, & \ldots & ,e_k\rangle & & \end{array}$$

We have $\mu(s,v) = \sum_{1\le j\le k} c(e_j)$. For $i \in 1..k$ let v_i be the target node of e_i and define $t_0 = 0$ and $v_0 = s$. Then $d[v_i] \le \sum_{1\le j\le i} c(e_j)$ after time t_i as a simple induction shows. This is clear for $i = 0$ since $d[s]$ is initialized to zero and d-values are only decreased. After the relaxation of $e_i = R[t_i]$ for $i > 0$, we have $d[v_i] \le d[v_{i-1}] + c(e_i) \le \sum_{1\le j\le i} c(e_j)$. Thus after time t_k, we have $d[v] \le \mu(s,v)$. Since $d[v]$ cannot go below $\mu(s,v)$ by Lemma 26, we have $d[v] = \mu(s,v)$ after time t_k and hence after performing all relaxations in R.

Let us next prove that the *parent* information traces out shortest paths. We do so under the additional assumption that shortest paths are unique and leave the general case to the reader. After the relaxations in R, we have $d[v_i] = \mu(s,v_i)$ for $1 \le i \le k$. When $d[v_i]$ was set to $\mu(s,v_i)$ by an operation $\mathit{relax}(u,v_i)$, the existence of a path of length $\mu(s,v_i)$ from s to v_i was established. Since, by assumption, the shortest path from s to v_i is unique, we must have $u = v_{i-1}$ and hence $\mathit{parent}[v_i] = v_{i-1}$.

Exercise 173. Redo the second paragraph in the proof above, but without the assumption that shortest paths are unique.

Exercise 174. Let ES be the edges of G in some arbitrary order and let $ES^{(n-1)}$ be $n-1$ copies of ES. Show $\mu(s,v) = d[v]$ for all nodes v with $\mu(s,v) \ne -\infty$ after performing the relaxations $ES^{(n-1)}$.

In the next sections, we will exhibit more efficient sequences of relaxations for acyclic graphs and graphs with non-negative edge weights. We come back to general graphs is Section 10.5.

10.2 Directed Acyclic Graphs (DAGs)

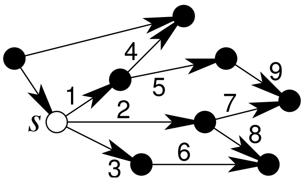


Fig. 10.3. Order of edge relaxations for shortest path computations from node s in a DAG. The topological order of nodes is given by their x-coordinate.

In a DAG, there are no directed cycles and hence no negative cycles. Moreover, we have learned in Section 9.2.1 that the nodes of a DAG can be topologically sorted into a sequence $\langle v_1, v_2, \ldots, v_n\rangle$ such that $(v_i, v_j) \in E$ implies $i < j$. A topological order can be computed in linear time $\mathcal{O}(n+m)$ using either depth-first search or breadth-first search. The nodes on any path in a DAG are increasing in topological

```
Dijkstra's Algorithm
declare all nodes unscanned and initialize $d$ and $parent$
while there is an unscanned node with tentative distance $< +\infty$ do
    $u$:= the unscanned node with minimal tentative distance
    relax all edges $(u, v)$ out of $u$ and declare $u$ scanned
```

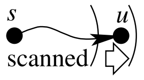


Fig. 10.4. Dijkstra's shortest path algorithm for non-negative edge weights

order. Thus, by Lemma 27, we compute correct shortest path distances if we first relax the edges out of v_1, then the edges out of v_2, etc, see Figure 10.3 for an example. In this way, each edge is relaxed only once. Since every edge relaxation takes constant time, we obtain a total execution time of $\mathcal{O}(m + n)$.

Theorem 27. *Shortest paths in acyclic graphs can be computed in time* $\mathcal{O}(n + m)$.

Exercise 175 (Route Planning for Public Transportation.). Finding quickest routes in public transportation systems can be modeled as a shortest path problem in acyclic graphs. Consider a bus or train leaving place p at time t and reaching its next stop p' at time t'. This connection is viewed as an edge connecting nodes (p, t) and (p', t'). Also, for each stop p and subsequent events (arrival and/or departure) at p, say at times t and t' with $t < t'$, we have the *waiting link* from (p, t) to (p, t'). (a) Show that the graph obtained in this way is a DAG. (b) You need an additional node modeling your starting point in space and time. There should also be one edge connecting it to the transportation network. How should this edge look? (c) Suppose you have computed the shortest path tree from your starting node to all nodes in the public transportation graph reachable from it. How do you actually find the route you are interested in?

10.3 Non-Negative Edge Costs (Dijkstra's Algorithm)

We now assume that all edge costs are non-negative. Thus there are no negative cycles and shortest paths exist for all nodes reachable from s. We will show that if the edges are relaxed in a judicious order, every edge needs to be relaxed only once.

What is the right order? Along any shortest path, the shortest path distances increase (more precisely, do not decrease). This suggests to scan nodes (to scan a node means to relax all edges out of the node) in order of increasing shortest path distance. Lemma 27 tells us that this relaxation order ensures the computation of shortest paths. Of course, in the algorithm we do not know shortest path distances, we only know the *tentative distances* $d[v]$. Fortunately, for the unscanned node with minimal tentative distance, true and tentative distance agree. We will prove this in Theorem 28. We obtain the algorithm shown in Figure 10.4. The algorithm is known as Dijkstra's shortest path algorithm. Figure 10.5 shows an example run.

operation	queue
$\mathit{insert}(s)$	$\langle(s,0)\rangle$
$\mathit{deleteMin}\rightsquigarrow (s,0)$	$\langle\rangle$
$\mathit{relax}\ s \xrightarrow{2} a$	$\langle(a,2)\rangle$
$\mathit{relax}\ s \xrightarrow{10} d$	$\langle(a,2),(d,10)\rangle$
$\mathit{deleteMin}\rightsquigarrow (a,2)$	$\langle(d,10)\rangle$
$\mathit{relax}\ a \xrightarrow{3} b$	$\langle(b,5),(d,10)\rangle$
$\mathit{deleteMin}\rightsquigarrow (b,5)$	$\langle(d,10)\rangle$
$\mathit{relax}\ b \xrightarrow{2} c$	$\langle(c,7),(d,10)\rangle$
$\mathit{relax}\ b \xrightarrow{1} e$	$\langle(e,6),(c,7),(d,10)\rangle$
$\mathit{deleteMin}\rightsquigarrow (e,6)$	$\langle(c,7),(d,10)\rangle$
$\mathit{relax}\ e \xrightarrow{9} b$	$\langle(c,7),(d,10)\rangle$
$\mathit{relax}\ e \xrightarrow{8} c$	$\langle(c,7),(d,10)\rangle$
$\mathit{relax}\ e \xrightarrow{0} d$	$\langle(d,6),(c,7)\rangle$
$\mathit{deleteMin}\rightsquigarrow (d,6)$	$\langle(c,7)\rangle$
$\mathit{relax}\ d \xrightarrow{4} s$	$\langle(c,7)\rangle$
$\mathit{relax}\ d \xrightarrow{5} b$	$\langle(c,7)\rangle$
$\mathit{deleteMin}\rightsquigarrow (c,7)$	$\langle\rangle$

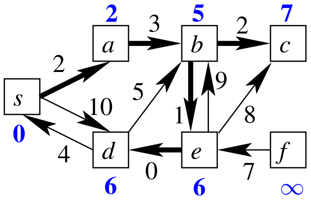


Fig. 10.5. Example run of Dijkstra's algorithm on the graph given to the right. The bold edges form the shortest path tree and the numbers in bold indicate shortest path distances.
The table above illustrates the execution. The queue consists of all pairs $(v, d[v])$ with v reached and unscanned. Initially, s is reached and unscanned. The actions of the algorithm are given in the first and third column. The second and fourth column show the state of the queue after the action.

Note that Dijkstra's algorithm is basically the thread-and-knot algorithm we saw in the introduction of this chapter: Suppose we put all threads and knots on a table and then lift up the starting node. The other knots will leave the surface of the table in the order of their shortest path distance.

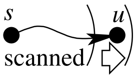
Theorem 28. *Dijkstra's algorithm solves the single-source shortest paths problem for graphs with non-negative edge costs.*

Proof. Assume that the algorithm is incorrect and consider the first time that we scan a node with its tentative distance larger than its shortest path distance. Say at time t we scan node v with $\mu(s,v) < d[v]$. Let $p = \langle s = v_1, v_2, \ldots, v_k = v\rangle$ be a shortest path from s to v and let i be minimal such that v_i is unscanned just before time t. Then $i > 0$ since s is the first node scanned (in the first iteration s is the only node whose tentative distance is less than $+\infty$) and $\mu(s,s) = 0 = d[s]$ when s is scanned. Thus v_{i-1} was scanned before time t and hence $d[v_{i-1}] = \mu(s, v_{i-1})$ when v_{i-1} was scanned (by definition of t[ps: geklammert. Immer noch etwas unschoen]). ⟸ When v_{i-1} was scanned, $d[v_i]$ was set to $\mu(s,v_{i-1}) + c(v_{i-1}, v_i) = \mu(s, v_i)$. Thus $d[v_i] = \mu(s,v_i) \le \mu(s,v_k) < d[v_k]$ just before time t and hence v_i is scanned instead of v_k, a contradiction.

Exercise 176. Let $v_1, v_2, \ldots$ be the order in which nodes are scanned. Show $\mu(s,v_1) \le \mu(s,v_2) \le \ldots$, i.e., nodes are scanned in order of increasing shortest path distances.

Exercise 177 (Verification of shortest path distances). Assume that all edge costs are positive, that all nodes are reachable from s, and that d is a node array of non-negative reals satisfying $d[s] = 0$ and $d[v] = \min_{(u,v)\in E} d[u] + c(u,v)$ for $v \ne s$. Show $d[v] = \mu(s,v)$ for all v.

```
Function Dijkstra(s : NodeId) : NodeArray×NodeArray
    d = ⟨∞, ..., ∞⟩ : NodeArray of ℝ ∪ {∞}                 // tentative distance from root
    parent = ⟨⊥, ..., ⊥⟩ : NodeArray of NodeId
    parent[s] := s                                          // self-loop signals root
    Q : NodePQ                                              // unscanned reached nodes
    d[s] :=0;   Q.insert(s)
    while $Q \neq \emptyset$ do
        u :=Q.deleteMin                                     // we have $d[u] = \mu(s,u)$

        foreach edge $e = (u, v) \in E$ do
            if $d[u] + c(e) < d[v]$ then                     // relax
                $d[v] := d[u] + c(e)$
                parent[v] :=u                               // update tree
                if $v \in Q$ then Q.decreaseKey(v)
                else Q.insert(v)
    return (d, parent)
```



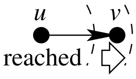


Fig. 10.6. Pseudocode for Dijkstra's Algorithm.

⟹ ***Exercise 178** [gesternt] Extend the statement of the previous exercise to non-negative cost functions. Be careful.

We come to the implementation of Dijkstra's algorithm. The crucial operation is finding the unscanned reached node with minimum tentative distance value. The addressable priority queues from Section 6.2 are the appropriate data structure. We store all unscanned reached nodes in an addressable priority queue using their tentative distance values as keys. The $deletemin$ returns the unscanned reached node with minimal distance. We also have a $NodeArray$ A. For each unscanned reached node v, $A[v]$ stores the handle to the item representing v in the addressable priority queue. For all other nodes, $A[v]$ is nil. We call the combination of addressable priority queue and node array a $NodePQ$. An $insert(v)$ adds an item for v with key $d[v]$ to the queue and stores the handle to the item in $A[v]$. A $deleteMin$ returns the node in the queue with minimal d-value, deletes the corresponding item from the queue, and sets $A[v]$ to nil. Finally, $decreaseKey(v)$ uses $A[v]$ to access the item for v and updates the addressable priority queue so as to reflect the new value of $d[v]$. The node array A can be implemented in different ways as discussed in Chapter **??**. For example, we may use an array indexed by node ids or incorporate space for the handle into the node objects.

We obtain the algorithm given in Figure 10.6. We next analyze its running time in terms of the running times for the queue operations. Initializing the arrays d and $parent$ and setting up a priority queue $Q = \{s\}$ takes time $\mathcal{O}(n)$. Checking for $Q = \emptyset$ and loop control takes constant time per iteration of the while-loop, i.e., $\mathcal{O}(n)$ time in total. Every node reachable from s is removed from the queue exactly once. Every reachable node is also $insert$ed exactly once. Thus we have at most n $deleteMin$ and $insert$ operations. Since each node is scanned at most once, each edge is relaxed at most once and hence there can be at most m *decreaseKey* operations. We obtain a total execution time of

$$T_{\text{Dijkstra}} := \mathcal{O}(n \cdot (T_{deleteMin}(n) + T_{insert}(n)) + m \cdot T_{decreaseKey}(n)) \,,$$

where $T_{deleteMin}$, T_{insert}, $T_{decreaseKey}$ denote the execution time for *deleteMin*, *insert*, and *decreaseKey*, respectively. Note that these execution times are a function of the queue size $|Q| = \mathcal{O}(n)$.

Exercise 179. Design a graph and a non-negative cost function such that the relaxation of $m - (n-1)$ edges causes a *decreaseKey* operation.

In his original 1959 paper, Dijkstra proposed the following implementation of the priority queue:[ps: reformulated to avoid double 'propose'] Maintain the number ⟸ of reached unscanned nodes and two arrays indexed by nodes — an array d storing the tentative distances and an array storing for each node whether it is unscanned or reached. Then *insert* and *decreaseKey* take time $O(1)$. A *deleteMin* takes time $O(n)$ since it has to scan the arrays in order to find the minimum tentative distance of any reached unscanned node. Thus total running time becomes

$$T_{Dijkstra59} = O(m + n^2) \ .$$

Much better priority queue implementations were invented since Dijkstra's original paper. With the binary heap and Fibonacci heap priority queues from Section 6.2 we obtain[ps: added 'respectively', aligned] ⟸

$$\begin{aligned} T_{DijkstraBHeap} &= O((m+n)\log n) \\ T_{DijkstraFibonacchi} &= O(m + n\log n) \text{ respectively.} \end{aligned}$$

Asymptotically, the Fibonacci heap implementation is superior except for sparse graphs with $m = O(n)$. In practice, Fibonacci heaps are usually not the fastest implementation because they involve larger constant factors and since the actual number of decrease key operations tends to be much smaller than what the worst case predicts. This experimental observation is supported by theoretical analysis. We will show that the expected number of *decreaseKey* operations is $\mathcal{O}(n \log(m/n))$.

Our model of randomness is as follows: the graph G and the source nodes s are arbitrary. Also, for each node v, we have an arbitrary set $C(v)$ of $indegree(v)$ non-negative real numbers. So far, everything is arbitrary. The randomness comes now: we assume that for each v the costs in $C(v)$ are assigned randomly to the edges *into* v, i.e., our probability space consists of $\prod_{v \in V} indegree(v)!$ many assignments of edge costs to edges. We want to stress that this model is quite general. In particular, it covers the situation that edges costs are drawn independently from a common distribution.

Theorem 29. *Under the assumptions above, the expected number of decreaseKey operations is* $O(n \log \frac{m}{n})$.

Proof. We present a proof due to Noshita [144]. Consider a particular node v and let $k = \mathit{indegree}(v)$. In any run of Dijkstra's algorithm, the edges into v are relaxed in some particular order, say $e_1, \ldots, e_k$. Let $e_i = (u_i, v)$. It is crucial to observe that the order in which the edges into v are relaxed does not depend on how the costs in $C(v)$ are assigned to the edges into v. We have $d[u_1] \leq d[u_2] \leq \ldots \leq d[u_k]$ since nodes are scanned in increasing order of tentative distances; here $d[u_i]$ is the tentative (and hence true) distance of u_i when u_i is scanned. If e_i causes a $\mathit{decreaseKey}$ operation then

$$d[u_i] + c(e_i) < \min_{j<i} d[u_j] + c(e_j) \ .$$

Since $d[u_i] \leq d[u_j]$, this implies

$$c(e_i) < \min_{j<i} c(e_j),$$

i.e., only left-right minima of the sequence $c(e_1)$,...,$c(e_k)$ can cause $\mathit{decreaseKey}$ operations. We conclude that the number of $\mathit{decreaseKey}$ operations on v is bounded by the number of left-right minima in the sequence $c(e_1)$,...,$c(e_k)$ minus one; the -1 accounts for the fact that the first element in the sequence counts as a left-right minimum but causes an insert and no $\mathit{decreaseKey}$. In Section 2.8 we have shown that the expected number of left-right maxima in a permutation of size k is bounded by H_k. The same bound holds for minima. Thus the expected number of $\mathit{decreaseKey}$ operations is bounded by $H_k - 1$ which in turn is bounded by $\ln k$. Summing over all nodes, we obtain the following bound for the expected number of $\mathit{decreaseKey}$ operations:

$$\sum_{v \in V} \ln \mathit{indegree}(v) \leq n \ln \frac{m}{n} \ ,$$

where the last inequality follows from the concavity of the ln-function (see Equation (A.16)). [todo: ueberall endofbeweis richtig machen] $\Longrightarrow$

We conclude that the expected running time is $O(m+n\log(m/n)\log n)$ with the binary heap implementation of priority queues. For sufficiently dense graphs ($m > n \log n \operatorname{loglog} n$) we will obtain execution time linear in the size of the input.

Exercise 180. Show that $\mathrm{E}[T_{\mathit{DijkstraBHeap}}] = \mathcal{O}(m)$ if $m = \Omega(n \log n \operatorname{loglog} n)$.

10.4 Monotone Integer Priority Queues

Dijkstra's algorithm does not really need a general purpose priority queue. It only requires what is known as a monotone priority queue. The usage of a priority queue is monotone if the sequence of deleted elements has non-decreasing keys. Dijkstra's algorithm uses its queue in a monotone way because insert and $\mathit{decreaseKey}$ operations use distances of the form $d[u] + c(e)$ where $d[u]$ is the key value of the last $\mathit{deleteMin}$ and $c(e)$ is a non-negative edge cost.

It is not known whether monotonicity can be exploited in the case of general real edge costs. However, for integer edge costs significant savings are possible. We therefore assume for this section that edges costs are integers in the range $0..C$ for some integer C. C is assumed to be known when the queue is initialized.

Since a shortest path can consist of at most $n-1$ edges, shortest path distances are at most $(n-1)C$. The range of values in the queue at any one time is even smaller. Let min be the last value deleted from the queue (zero before the first deletion). Dijkstra's algorithm maintains the invariant that all values in the queue are contained in $\mathit{min}..\mathit{min}+C$. The invariant certainly holds after the first insertion. A $\mathit{deleteMin}$ may increase min. Since all values in the queue are bounded by C plus the old value of min, this is certainly true for the new value of min. Edge relaxations insert priorities of the form $d[u]+c(e)=\mathit{min}+c(e)\in \mathit{min}..\mathit{min}+C$.

10.4.1 Bucket Queues

A bucket queue is a circular array B of $C+1$ doubly linked lists (see Figure 10.7 and also Algorithm 3.8). We view the natural numbers wrapped around the circular array, all integers of the form $i+(C+1)j$ map to index i. A node $v\in Q$ with tentative distance $d[v]$ is stored in $B[d[v] \bmod (C+1)]$. Since the priorities in the queue are contained in $\mathit{min}..\mathit{min}+C$ at any one time, all nodes in a bucket have the *same* distance value.

Initialization creates $C+1$ empty lists. An $\mathit{insert}(v)$ inserts v into $B[d[v] \bmod C+1]$. A $\mathit{decreaseKey}(v)$ removes v from the list containing it and inserts it into $B[d[v] \bmod C+1]$. Thus insert and $\mathit{decreaseKey}$ take constant time if buckets are implemented as doubly linked lists.

A $\mathit{deleteMin}$ first looks at bucket $B[\mathit{min} \bmod C+1]$. If this bucket is empty, it increments min and repeats. In this way the total cost of all $\mathit{deleteMin}$ operations is $O(n+nC)=\mathcal{O}(nC)$ since min is incremented at most nC times and since at most n elements are deleted from the queue. Plugging the operation costs for the bucket queue implementation with integer edge costs in $0..C$ into our general bound for the cost of Dijkstra's algorithm we obtain:

$$T_{\text{DijkstraBucket}}=\mathcal{O}(m+nC) \quad .$$

***Exercise 181 (Dinitz' Refinement of Bucket Queues [58].)** Assume edge costs are positive real numbers in $[c_{\min},c_{\max}]$. Explain how to find shortest paths in time $\mathcal{O}(m+nc_{\max}/c_{\min})$. Hint: use Buckets of width $c_{\min}$. Show that all nodes in the smallest non-empty bucket have $d[v]=\mu(s,v)$.

10.4.2 Radix Heaps

Radix heaps improve on the bucket queue implementation by using buckets of different width. Narrow buckets are used for tentative distances close to min and wide buckets are used for tentative distances far away from min. In this section we will show how this approach leads to a version of Dijkstra's algorithm with running time

$$T_{\text{DijkstraRadix}}:=\mathcal{O}(m+n\log C) \quad .$$

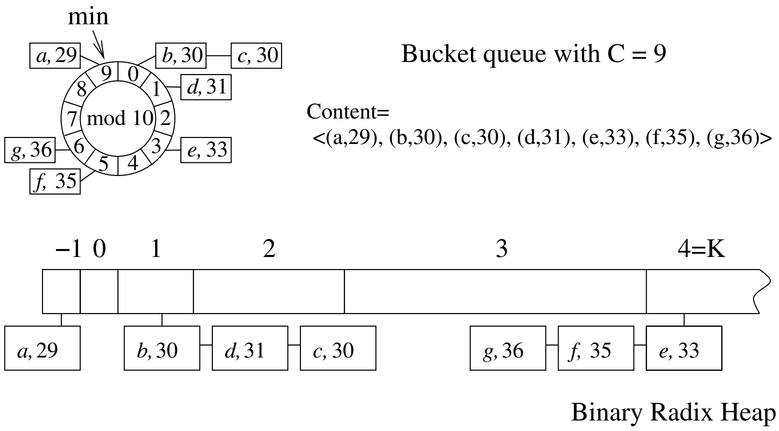


Fig. 10.7. Example for a bucket queue and a radix heap. The upper part shows a bucket queue with content $\langle(a, 29), (b, 30), (c, 30), (d, 31), (e, 33), (f, 35), (g, 36)\rangle$, $C = 9$, and $min = 29$. The lower part shows the corresponding bucket heap. The binary representation of 29 is 11101. Also, we have $K = 1 + \lceil \log C \rceil = 4$. Therefore, bucket $B[-1]$ contains all nodes with d-value equal to 29, $B[0]$ is empty, $B[1]$ contains all nodes whose d-value has a representation of the form 1111*, i.e., d-value 30 or 31, buckets $B[2]$ and $B[3]$ are empty, and bucket $B[4]$ contains all nodes whose d-value has a binary representation containing a one in position 4 or higher, i.e., d-value 32 or larger.

Radix heaps exploit the binary representation of tentative distances. We need the concept of the *most significant distinguishing index* of two numbers. It is the largest index where the binary representations differ, i.e., for numbers a and b with binary representations $a = \sum_{i \geq 0} \alpha_i 2^i$ and $b = \sum_{i \geq 0} \beta_i 2^i$ define the most significant distinguishing index $msd(a, b)$ as the largest i with $\alpha_i \neq \beta_i$ and let it be -1 if $a = b$. If $a < b$ then a has a zero bit in position $i = msd(a, b)$ and b has a one bit.

A radix heap consists of an array of buckets $B[-1]$, $B[0]$, ..., $B[K]$ where $K = 1 + \lfloor \log C \rfloor$. The queue elements are distributed over the buckets according to the following rule:

$$\text{any queue element } v \text{ is stored in bucket } B[i] \text{ where } i = \min(msd(min, d[v]), K).$$

We refer to this rule as the bucket queue invariant. Figure 10.7 illustrates the bucket queue invariant. We remark that if min has a one bit in position i for $0 \leq i < K$, the corresponding bucket $B[i]$ is empty. This holds since any $d[v]$ with $i = msd(min, d[v])$ would have a zero bit in position i and hence be smaller than min. But all keys in the queue are at least as large as min.

How can we compute $i := msd(a, b)$? We first observe, that for $a \neq b$, the bitwise exclusive-or $a \oplus b$ of a and b has its most significant one in position i and hence represents an integer whose value is at least 2^i and less than 2^{i+1}. Thus $msd(a, b) = \lfloor \log(a \oplus b) \rfloor$, since $\log(a \oplus b)$ is a real number with integer part equal to i and the floor function extracts the integer part. Many processors support the computation of msd by machine instructions[2]. Alternatively, we can use look-up tables or yet different solutions. From now on we will assume that msd can be evaluated in constant time.

We turn to the queue operations. Initialization, $insert$, and $decreaseKey$ work completely analogously to bucket queues with the only difference being that they use the bucket queue invariant to compute bucket indices.

A $deleteMin$ first finds the minimum i such that $B[i]$ is non-empty. If $i = -1$, an arbitrary element in $B[-1]$ is removed and returned. If $i \geq 0$, the bucket $B[i]$ is scanned and min is set to the smallest tentative distance contained in the bucket. Since min has changed, the bucket queue invariant needs to be restored. A crucial observation for the efficiency of radix heaps is that only the nodes in bucket i are affected. We will discuss below, how they are affected. Let us first consider the buckets $B[j]$ with $j \neq i$. Buckets $B[j]$, with $j < i$ are empty. If $i = K$, there are no j with $j > K$. If $i < K$, any key a in bucket $B[j]$ with $j > i$ will still have $msd(a, min) = j$, because the old and new values of min agree on bit positions greater than i.

What happens to the elements in $B[i]$? Its elements are moved to the appropriate new bucket. Thus a $deleteMin$ takes constant time if $i = -1$ and takes time $O(i + |B[i]|) = O(K + |B[i]|)$ if $i \geq 0$. Lemma 28 below shows that every node in bucket $B[i]$ is moved to a bucket with a smaller index. This observation allows us to account for the cost of a $deleteMin$ using amortized analysis. As our unit of cost (one token) we will use the time required to move one node between buckets.

We charge $K + 1$ tokens to operation $insert(v)$ and associate the K tokens with v. These tokens pay for the moves of v to lower number buckets in $deleteMin$ operations. A node starts in some bucket j with $\leq K$, ends in bucket -1, and in between never moves back to a higher numbered bucket. Observe, that a $decreaseKey(v)$ operation will also never move a node to a higher number bucket. Hence, the $K + 1$ tokens can pay for all the node moves of $deleteMin$ operations. The remaining cost of a $deleteMin$ is $\mathcal{O}(K)$ for finding a non-empty bucket. With amortized cost $K + 1 + \mathcal{O}(1) = \mathcal{O}(K)$ for an $insert$ and $\mathcal{O}(1)$ for a $decreaseKey$, we obtain a total execution time of $\mathcal{O}(n \cdot (K + K) + m) = \mathcal{O}(m + n \log C)$ for Dijkstra's algorithm as claimed.

It remains to prove that $deleteMin$ operations move nodes to lower numbered buckets.

Lemma 28. *Let i be minimal such that $B[i]$ is non-empty and assume $i \geq 0$. Let min be the smallest element in $B[i]$. Then $msd(min, x) < i$ for all $x \in B[i]$.*

Proof. First observe that the case $x = min$ is easy since $msd(x, x) = -1 < i$. For the non-trivial case $x \neq min$ we distinguish the subcases $i < K$ and $i = K$. Let min_o be the old value of min. Figure 10.8 shows the structure of the relevant keys. **Case $i < K$:** The most significant distinguishing index of min_o and any $x \in B[i]$

[2] $\oplus$ is a direct machine instruction and $\lfloor \log x \rfloor$ is the exponent in the floating point representation of x.

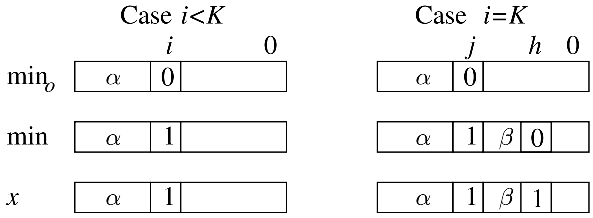


Fig. 10.8. The structure of the keys relevant for the proof of Lemma 28. In the proof it is shown that β starts with $j - K$ zeroes.

is i, i.e., min_o has a zero in bit position i and all $x \in B[i]$ have a one in bit position i. They agree in all positions with index larger than i. Thus the most significant distinguishing index for min and x is smaller than i.

Case $i = K$: Consider any $x \in B[K]$. Let $j = msd(min_o, min)$. Then $j \geq K$ since $min \in B[K]$. Let $h = msd(min, x)$. We want to show $h < K$. Let α comprise the bits in positions larger than j in min_0 and let A be the number obtained from min_o by setting the bits in positions 0 to j to zero. Then α followed by $j + 1$ zeroes is the binary representation of A. Since the j-th bit of min_o is zero and is one for min we have $min_0 < A + 2^j$ and $A + 2^j \leq min$. Also, $x \leq min_o + C < A + 2^j + C \leq A + 2^j + 2^K$. So

$$A + 2^j \leq min \leq x < A + 2^j + 2^K$$

and hence the binary representations of min and x consist of the binary representation of A followed by a 1, followed by $j - K$ zeroes, followed by some bitstring of length K. Thus min and x agree in all bits with index K or larger and hence $h < K$.

In order to aid intuition, we give a second proof for the case $i = K$[ps
$\Longrightarrow$ was:$i = KK$???]. We first observe that the binary representation of min starts with α followed by a one. We next observe that x can be obtained from min_0 by adding some K-bit number. Since $min \leq x$, the final carry in this addition must run into position j. Otherwise, the j-th bit of x would be zero and hence $x < min$. Since min_0 has a zero in position j, the carry stops in position j. We conclude that the binary representation of x is equal to α followed by a 1, followed by $j - K$ zeroes followed by some K bit string. Since $min \leq x$, the $j - K$ zeroes must also be present in the binary representation of min.

***Exercise 182** Radix heaps can also be based on number representations with base b for any $b \geq 2$. In this situation we have buckets $B[i, j]$ for $i = -1, 0, 1, \ldots K$ and $0 \leq j \leq b$, where $K = 1 + \lfloor \log C / \log b \rfloor$. An unscanned reached node x is stored in bucket $B[i, j]$ if $msd(min, d[x]) = i$ and the i-th digit of $d[x]$ is equal to j. We also store for each i, the number of nodes contained in buckets $\cup_j B[i, j]$. Discuss the implementation of the priority queue operations and show that a shortest path algorithm with running time $O(m + n(b + \log C / \log b))$ results. What is the optimal choice of b?

If the edge costs are random integers in the range $0..C$, a small change of the algorithm guarantees linear running time [133, 75]. For every node v, let $c_{\min}^{\text{in}}(v)$ denote the minimum cost of an incoming edge. We divide Q into two parts, a part F which contains unscanned nodes whose tentative distance label is known to be equal to their exact distance from s, and a part B which contains all other reached unscanned nodes. B is organized as a radix heap. We also maintain a value min. We scan nodes as follows.

When F is non-empty, an arbitrary node in F is removed and the outgoing edges are relaxed. When F is empty, the minimum node is selected from B and min is set to its distance label. When a node is selected from B, the nodes in the first non-empty bucket $B[i]$ are redistributed if $i \geq 0$. There is a small change in the redistribution process. When a node v is to be moved, and $d[v] \leq \mathit{min} + c_{\min}^{\text{in}}(v)$, we move v to F. Observe that any future relaxation of an edge into v cannot decrease $d[v]$ and hence $d[v]$ is known to be exact at this point.

The algorithm is correct since it is still true that $d[v] = \mu(s, v)$ when v is scanned. For nodes removed from F this was argued in the previous paragraph and for nodes removed from B this follows from the fact that they have the smallest tentative distance among all unscanned reached nodes.

Theorem 30. *Let G be an arbitrary graph and let c be a random function from E to $0..C$. Then the single-source problem can be solved in expected time $O(n + m)$.*

Proof. We still need to argue the bound on the running time. We modify the amortized analysis of plain radix heaps. As before, nodes start out in $B[K]$. When a node v is moved to a new bucket, but not yet to F, $d[v] > \mathit{min} + c_{\min}^{\text{in}}(v)$ and hence v is moved to a bucket $B[i]$ with $i \geq \log c_{\min}^{\text{in}}(v)$. Hence, it suffices if insert pays $K - \log c_{\min}^{\text{in}}(v) + 1$ tokens into the account for node v in order to cover all costs due to $\mathit{decreaseKey}$ and $\mathit{deleteMin}$ operations operating on v. Summing over all nodes we obtain a total payment of

$$\sum_v (K - \log c_{\min}^{\text{in}}(v) + 1) = n + \sum_v (K - \log c_{\min}^{\text{in}}(v)) .$$

We need to estimate the sum. For each vertex, we have one incoming edge contributing to this sum. We therefore bound the sum from above, if we sum over all edges, i.e.,

$$\sum_v (K - \log c_{\min}^{\text{in}}(v)) \leq \sum_e (K - \log c(e)) .$$

$K - \log c(e)$ is the number of leading zeros in the binary representation of $c(e)$ when written as a K-bit number. Our edge costs are uniform random numbers in $0..C$ and $K = 1 + \lfloor \log C \rfloor$. Thus $\text{prob}(K - \log c(e)) = i) = 2^{-i}$. Using Equation (A.14) we conclude

$$\mathrm{E}\left[\sum_e (k - \log c(e))\right] = \sum_e \sum_{i \geq 0} i 2^{-i} = O(m).$$

Thus the total expected cost of $\mathit{deleteMin}$ and $\mathit{decreaseKey}$ operations is $O(n+m)$. The time spent outside these operations is also $O(n + m)$.

```
Function BellmanFord(s : NodeId) : NodeArray×NodeArray
    d = $\langle\infty,\ldots,\infty\rangle$ : NodeArray of $\mathbb{R}\cup\{-\infty,\infty\}$        // distance from root
    parent = $\langle\bot,\ldots,\bot\rangle$ : NodeArray of NodeId
    $d[s] := 0$;   $parent[s] := s$                                  // self-loop signals root
    for $i := 1$ to $n-1$ do
        forall $e \in E$ do relax($e$)                                      // round $i$
    forall $e = (u,v) \in E$ do                                          // postprocessing
        invariant $\forall v \in V : d[v] = -\infty \to \forall w$ reachable from $v : d[w] = -\infty$
        if $d[u] + c(e) < d[v]$ then infect($v$)
    return $(d, parent)$

Procedure infect($v$)
    if $d[v] > -\infty$ then
        $d[v] := -\infty$
        foreach $(v,w) \in E$ do infect($w$)
```

Fig. 10.9. The Bellman-Ford algorithm for shortest paths in arbitrary graphs.

It is a bit odd that the maximum edge cost C appears in the premise, but not in the conclusion of Theorem 30. Indeed, it can be shown that a similar result holds for random real valued edge costs.

****Exercise 183** Explain how to adapt the above algorithm for the case that c is a random function from E to the real interval $(0,1]$. The expected time should still be $O(n+m)$. What assumptions do you need on the representation of edge costs and on the machine instructions available? Hint: you may first want to solve Exercise 181. The most narrow bucket should have width $\min_{e\in E} c(e)$. Subsequent buckets have geometrically growing widths.

10.5 Arbitrary Edge Costs (Bellman-Ford Algorithm)

For acyclic graphs and for non-negative edge costs we got away with m edge relations. For arbitrary edge costs no such result is known. However, it is easy to guarantee the correctness criterion of Lemma 27 using $\mathcal{O}(n \cdot m)$ edge relaxations: the Bellman-Ford algorithm given in Figure 10.9 performs $n-1$ rounds. In each round it relaxes all edges. Since simple paths consist of at most $n-1$ edges, every shortest path is a subsequence of this sequence of relaxations. Thus after the relaxations are completed, we have $d[v] = \mu(s,v)$ for all v with $-\infty < d[v] < \infty$ by Invariant 2. Moreover, $parent$ encodes the shortest paths to these nodes. Nodes v unreachable from s will still have $d[v] = \infty$ as desired.

It is not so obvious how to find the nodes v with $\mu(s,v) = -\infty$. Consider any edge $e = (u,v)$ with $d[u]+c(e) < d[v]$. We can set $d[v]:=-\infty$ because if there were a shortest path from s to v we would have found it by now and relaxing e would not lead to shorter distances any more. We can then also set $d[w] = -\infty$ for all nodes

w reachable from v. The pseudocode implements this approach using a recursive function $\mathit{infect}(v)$. It sets the d-value of v and all nodes reachable from it to $-\infty$. If infect reaches a node w that already has $d[w] = -\infty$, it breaks the recursion because previous executions of infect have already explored all nodes reachable from w. If $d[v]$ is not set to $-\infty$ during postprocessing, we have $d[x] + c(e) \geq d[y]$ for any edge $e = (x, y)$ on any path p from s to v. Thus $d[s] + c(p) \geq d[v]$ for any path p from s to v, and hence $d[v] \leq \mu(s, v)$. We conclude $d[v] = \mu(s, v)$.

Exercise 184. Show that postprocessing runs in time $\mathcal{O}(m)$. Hint: relate infect to DFS.

Exercise 185. Someone proposes an alternative postprocessing algorithm: set $d[v]$ to $-\infty$ for all nodes v for which following parents does not lead to s. Give an example, where this method overlooks a node with $\mu(s, v) = -\infty$.

Exercise 186 (Arbitrage.). Consider a set of currencies C with an exchange rate of r_{ij} between currencies i and j (you obtain r_{ij} units of currency j for one unit of currency i). A *currency arbitrage* is possible if there is a sequence of elementary currency exchange actions that starts with one unit of a currency and ends with more than one unit of the same currency. (a) Show how to find out whether a matrix of exchange rates admits currency arbitrage. Hint: $\log(xy) = \log x + \log y$. (b) Refine your algorithm so that it outputs a sequence of exchange steps that maximizes the average profit *per transaction*.

Section 10.9 outlines further refinements for Bellman-Ford that are necessary for good performance in practice.

10.6 All-Pairs Shortest Paths and Potential Functions

The all-pairs problem is tantamount to n single-source problems and hence can be solved in time $O(n^2 m)$. A considerable improvement is possible. We show that it suffices to solve one general single-source problem plus n single-source problems with non-negative edge costs. In this way, we obtain a running time of $O(nm + n(m + n \log n)) = O(nm + n^2 \log n)$. We need the concept of a potential function.

A *potential function* assigns a number $\mathit{pot}(v)$ to each node v. For an edge $e = (v, w)$ we define its *reduced cost* $\bar{c}(e)$ as:

$$\bar{c}(e) = \mathit{pot}(v) + c(e) - \mathit{pot}(w) \ .$$

Lemma 29. *Let p and q be paths from v to w. Then $\bar{c}(p) = \mathit{pot}(v) + c(p) - \mathit{pot}(w)$ and $\bar{c}(p) \leq \bar{c}(q)$ iff $c(p) \leq c(q)$. In particular, shortest paths with respect to $\bar{c}$ are the same as with respect to c.*

Proof. The second and the third claim follow from the first. For the first claim, let $p = \langle e_0, \ldots, e_{k-1} \rangle$ with $e_i = (v_i, v_{i+1})$, $v = v_0$ and $w = v_k$. Then

```
**All-Pairs Shortest Paths in the Absence of Negative Cycles**
add a new node $s$ and zero length edges $(s, v)$ for all $v$      // no new cycles, time $O(m)$
compute $\mu(s, v)$ for all $v$ with Bellman-Ford                  // time $O(nm)$
set $pot(v) = \mu(s, v)$ and compute reduced costs $\bar{c}(e)$ for $e \in E$      // time $O(m)$
forall nodes $x$ do                                                 // time $O(n(m + n \log n))$
    use Dijkstra's algorithm to compute the reduced shortest path distances $\bar{\mu}(x, v)$
    using source $x$ and the reduced edge costs $\bar{c}$
// translate distances back to original cost function              // time $O(m)$
forall $e = (v, w) \in V \times V$ do $\mu(v, w) := \bar{\mu}(v, w) + pot(w) - pot(v)$
```

Fig. 10.10. All-Pairs Shortest Paths in the Absence of Negative Cycles

$$\begin{aligned}\bar{c}(p) = \sum_{i=0}^{k-1} \bar{c}(e_i) &= \sum_{0 \leq i < k} (pot(v_i) + c(e_i) - pot(v_{i+1})) \\ &= pot(v_0) + \sum_{0 \leq i < k} c(e_i) - pot(v_k) = pot(v_0) + c(p) - pot(v_k) \,.\end{aligned}$$

Exercise 187. Potential functions can be used to generate graphs with negative edge costs but no negative cycles: generate a (random) graph, assign to every edge e a (random) non-negative (!!!) cost $c(e)$, assign to every node v a (random) potential $pot(v)$, and set the cost of $e = (u, v)$ to $\bar{c}(e) = pot(u) + c(e) - pot(v)$. Show that this rule does not generate negative cycles.

Lemma 30. *Assume that G has no negative cycles and that all nodes can be reached from s. Let $pot(v) = \mu(s, v)$ for $v \in V$. With this potential function reduced edge costs are non-negative.*

Proof. Since all nodes are reachable from s and since there are no negative cycles, $\mu(s, v) \in \mathbb{R}$ for all v. Thus the reduced costs are well defined. Consider an arbitrary edge $e = (v, w)$. We have $\mu(s, v) + c(e) \geq \mu(w)$ and hence $\bar{c}(e) = \mu(s, v) + c(e) - \mu(s, w) \geq 0$.

[ps: pseudocode von 10.10 deutlich umbeschrieben um undefinierte Symbole zu vermeiden. letze Zeile berechnete Abstaende nur fÃijr $(v, w) \in E$
$\Longrightarrow$???]

Theorem 31. *The all-pairs shortest paths problem in graphs without negative cycles can be solved in time $\mathcal{O}\big(nm + n^2 \log n\big)$.*

Proof. The algorithm is shown in Figure 10.10. We add an auxiliary node s and zero cost edges (s, v) for all nodes of the graph. This does not create negative cycles and does not change $\mu(v, w)$ for any of the existing nodes. Then we solve the single-source problem with source s and set $pot(v) = \mu(s, v)$ for all v. Next we compute reduced costs and then solve the single-source problem for each node v by means of Dijkstra's algorithm. Finally, we translate the computed distances back to the original cost function. The computation of the potentials takes time $\mathcal{O}(nm)$ and the n shortest path calculations take time $\mathcal{O}(n(m + n \log n))$. Pre- and postprocessing takes linear time.

The assumption that G has no negative cycles can be removed [128][ps: moved citation from further findings]. ⟸

Exercise 188. The *diameter* D of a graph G is defined as the largest distance between any two of its nodes. We can easily compute it using an all-pairs computation. Now we want to consider ways to *approximate* the diameter using a constant number of single-source computations. (a) For any starting node s, let $D'(s) := \max_{u \in V} \mu(s, u)$. Show that $D'(s) \leq D \leq 2D'(s)$ in undirected graphs. Also, show that no such relation holds in directed graphs. Let $D''(s) := \max_{u \in V} \mu(u, s)$. Show that $\max(D'(s), D''(s)) \leq D \leq D'(s) + D''(s)$ for undirected and directed graphs. (b) How should a graph be represented to support both forward and backward search? (c) Can you improve the approximation by considering more than one node s?

10.7 Shortest Path Queries

Often, we are interested in the shortest path from a specific source node s to a specific target node t; route planning in traffic networks is one such scenario. We will explain some techniques for solving such *shortest path queries* efficiently and argue their usefulness for the route planning application.

We start with a technique called *early stopping*. We run Dijkstra's algorithm to find shortest paths starting at s. We stop the search as soon as t is removed from the priority queue, because at this point in time the shortest path to t is known. This helps except for the unfortunate case when t is the farthest node from s. On average early stopping saves a factor of two in scanned nodes in any application. In practical route planning, early stopping saves much more because modern car navigation systems have a map of an entire continent but are mostly used for distances of a few hundred kilometers.

Another simple and general heuristic is *bidirectional search* from s forward and from t backward until the search frontiers meet. More precisely, we run two copies of Dijkstra's algorithm side by side, one starting from s and one starting from t (and running on the reversed graph). Each copy has its own queue, say Q_s and Q_t. We grow the search regions at about the same speed, for example, by removing a node from Q_s if $\min Q_s \leq \min Q_t$ and a node from Q_t, otherwise.

It is tempting to stop the search, once the first node u has been removed from both queues, and to claim that $\mu(s, t) = \mu(s, u) + \mu(u, t)$. Observe that execution of Dijkstra's algorithm on the reversed graph with starting node t determined $\mu(u, t)$. This is not quite correct, but almost so.

Exercise 189. Give an example, where u is *not* on the shortest path from s to t.

However, we have collected enough information once some node u has been removed from both queues. Let d_s and d_t denote the tentative distance labels in the runs

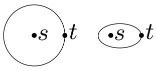


Fig. 10.11. Standard Dijkstra search grows a circular region centered at the source, goal-directed search grows a region leaning towards the target.

with source s and source t, respectively. Let $p = \langle s = v_0, \dots, v_i, v_{i+1}, \dots, v_k = t \rangle$ be a shortest path from s to t. Let i be maximal such that v_i was removed from Q_s. Then $d_s[v_{i+1}] = \mu(s, v_{i+1})$. Also, $\mu(s,u) \leq \mu(s, v_{i+1})$ since u was already removed from Q_s, but v_{i+1} was not. Next observe that

$$\mu(s, v_{i+1}) + \mu(v_{i+1}, t) = c(p) \leq \mu(s,u) + \mu(u,t) \ ,$$

since p is a shortest path from s to t. Thus

$$\mu(v_{i+1}, t) \leq \mu(s,u) + \mu(u,t) - \mu(s, v_{i+1}) \leq \mu(u,t)$$

and hence $d_t[v_{i+1}] = \mu(v_{i+1}, t)$ when the search stops. So we can determine the shortest distance from s to t by not only inspecting the first node removed from both queues, but all nodes in say Q_s. We iterate over all such nodes v and determine the minimum value of $d_s[v] + d_t[v]$.

Dijkstra's algorithm scans nodes in order of increasing distance from the source. In other words, it grows a circle centered at the source node. The circle is defined by the shortest path metric in the graph. In the route planning application in road networks, we may also consider geometric circles centered at the source and argue that shortest path circles and geometric circles are about the same. We can then estimate the speedup obtained by bidirectional search using the following heuristic argument: a circle of a certain diameter has twice the area of two circles of half the diameter. We could thus hope that bidirectional search saves a factor of two compared to unidirectional search.

Exercise 190 (Bidirectional Search). (a) Consider bidirectional search in a grid graph. How much does it save over unidirectional search? (b) Try to find a family of graphs where bidirectional search visits exponentially fewer nodes on the average than unidirectional search. Hint: consider random graphs or hypercubes. (c) Give an example where bidirectional search in real road networks takes *longer* than unidirectional search. Hint: consider a densely inhabitated city with sparsely populated surroundings. (d) Design a strategy for switching between forward and backward search such that bidirectional search will *never* inspect more than twice as many nodes as unidirectional search.

We will next describe two techniques that are more complex and less generally applicable, however, if applicable, usually result in larger savings. Both techniques mimic human behavior in route planning.

Goal-directed search: The idea is to bias the search space such that Dijkstra's algorithm does not grow a disc but a region protruding towards the target, see Figure 10.11. Assume, we know a function $f : V \to \mathbb{R}$ that estimates the distance to the target, i.e., $f(v)$ estimates $\mu(v,t)$ for all nodes v. We use the estimates to modify the distance function. For each $e = (u,v)$, let $\bar{c}(e) = c(e) + f(v) - f(u)$. We run Dijkstra's algorithm with the modified distance function. We know already that node potentials do not change shortest paths and hence correctness is preserved. Tentative distances are related via $\bar{d}[v] = d[v] + f(v) - f(s)$. An alternative view of this modification is that we run Dijkstra's algorithm with the original distance function but remove the node with minimal value $d[v] + f(v)$ from the queue. The algorithm just described is known as *A^*-search*.

Before we state requirements on the estimate f, let us see one specific example. Assume, for a Gedankenexperiment, $f(v) = \mu(v,t)$. Then $\bar{c}(e) = c(e) + \mu(v,t) - \mu(u,t)$ and hence edges on a shortest path from s to t have modified cost equal to zero and all other edges have positive cost. Thus Dijkstra's algorithm only follows shortest paths without looking left or right.

The function f must have certain properties to be useful. First, we want the modified distances to be non-negative. So we need, $c(e) + f(v) \geq f(u)$ for all edges $e = (u,v)$. In other words, our estimate for the distance from u should be at most our estimate for the distance from v plus the cost of going from u to v. This property is called consistency of estimates. [ps:reformulated sentence:]We also want to be $\Longleftarrow$ able to stop searching when t is removed from the queue. This works if f is a lower bound on the distance to the target, i.e., $f(v) \leq \mu(v,t)$ for all $v \in V$. Then $f(t) = 0$. Consider the point in time, when t is removed from the queue and let p be any path from s to t. If all edges of p have been relaxed at termination, $d[t] \leq c(p)$. If not all edges of p have been relaxed at termination, there is a node v on p that it contained in the queue at termination. Then

$$d[t] = d[t] + f(t) \leq d[v] + f(v) \leq d[v] + \mu(v,t) \leq c(p)\ ,$$

where the first inequality follows from the fact that t was removed before v. In either case, we have $d[t] \leq c(p)$ and hence the shortest distance from s to t is known as soon as t is removed from the queue.

What is a good heuristic function for route planning in road networks? Route planners often give the choice between *shortest* or *fastest* connections. In the case of shortest paths, a feasible lower bound $f(v)$ is the straight line distance between v and t. Speedups by a factor of roughly four are reported in literature. For fastest paths, we may use the geometric distance divided by the speed assumed for the best kind of road. This estimate is extremely optimistic, since targets are frequently in the center of town, and hence no good speed-ups are reported. More sophisticated methods for computing lower bounds are known; we refer the reader to [**?**] for a thorough discussion.

Hierarchy: Road networks usually know a hierarchy of roads: throughways, state roads, county roads, city roads, and so on. Average speed is usually higher on roads of higher status and therefore fastest routes frequently follow the pattern that one starts on a road of low status, keeps changing to roads of higher status, drives the largest fraction of the path on a road of high status and finally changes down to lower status roads near the target. A heuristic approach may therefore restrict the search to high-status roads except for neighborhoods of source and target. Observe however, that this heuristic sacrifices optimality. Try to think of an example from your driving experience where shortcuts over small roads are required even far away from source and target. Exactness can be combined with the idea of hierarchies if the hierarchy is defined algorithmically and is not taken from the official classification of roads. We outline one such approach [155], called *highway hierarchies*. It first defines a notion of locality, say anything within a distance of ten kilometers from either source or target. An edge $(u, v) \in E$ is a *highway edge* with respect to this notion of locality if there is a source node s and a target node t such that (u, v) is on the fastest path from s to t, v is not in the local search radius of s, and u is not in the local (backwards) search radius of t. The resulting network is called the *highway network*. It usually has many vertices of degree two. Think of a fast road into which a slow road connects. The slow road is not used on any fastest path outside the local region of source or target and hence will not be in the highway network. Thus the intersection will have degree three in the original road network, but will have degree two in the highway network. Two edges joined by a degree-two node may be collapsed into a single edge. In this way, the *core* of the highway network is determined. Iterating this procedure of finding a highway network and contracting degree-two nodes leads to a hierarchy of roads. For example, in the road networks of Europe and North America a hierarchy of up to ten levels resulted. Route planning using the resulting highway hierarchy can be several thousand times faster than Dijkstra's algorithm.

$\Longrightarrow$ [ps new paragraph:]

Transit Node Routing: Using another observation from daily life, we can get even faster [13]. When you drive to somewhere 'far away', you will leave your current location via one of only a few 'important' traffic junctions. It turns out that in real world road networks about 99 % of all quickest paths go through about $\mathcal{O}(\sqrt{n})$ important *transit nodes* that can be automatically selected, e.g., using highway hierarchies. Moreover, for each particular source or target node, all long distance connections go through about ten of these transit nodes — the *access nodes*. During preprocessing we compute a complete distance table between the transit nodes and the distances from all nodes to their access nodes. Now suppose we have a way to tell that source s and target t are sufficiently far apart[3]. Then there must be access nodes a_s and a_t such that $\mu(s,t) = \mu(s,a_s) + \mu(a_s,a_t) + \mu(a_t,t)$. All these distances have been precomputed and there are only about ten candidates for a_s and a_t respectably, i.e., we (only) need about 100 accesses to the distance table. This can be more than 1 000 000 times faster than Dijkstra's algorithm. Local queries can be answered using some other technique for which they are likely to be rather easy to handle, or we can cover them using additional procomputed tables with more local information. $\Longrightarrow$ Figure **??** gives an example[todo: Am Ende transitHighRes.ps verwenden].

[3] We may need additional preprocessing to decide this.

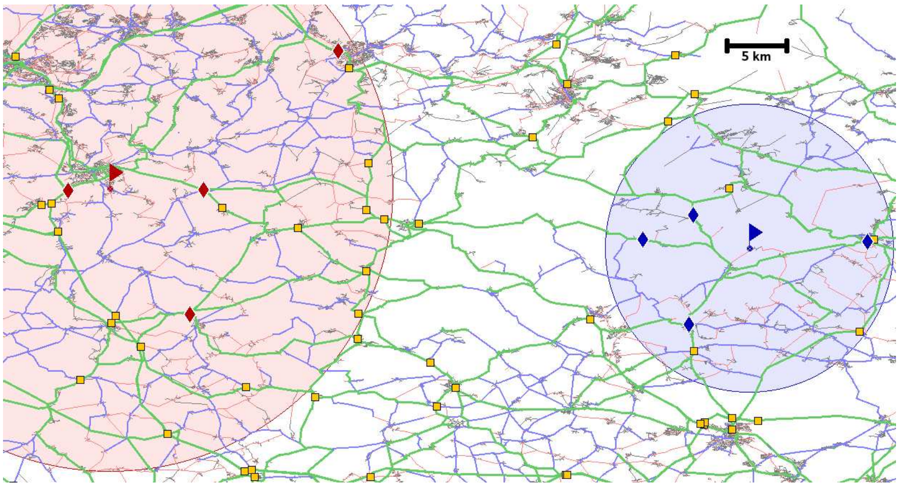


Fig. 10.12. Finding the optimal travel time between two points (the flags) somewhere between Saarbrücken and Karlsruhe amounts to retrieving the 2×4 *access nodes* (diamonds), performing 16 table lookups between all pairs of access nodes, and checking that the two disks defining the *locality filter* do not overlap. The small squares indicate further transit nodes.

10.8 Implementation Notes

Shortest path algorithms work over the set of extended reals $\mathbb{R} \cup \{+\infty, -\infty\}$. We may ignore $-\infty$ since it is only needed in the presence of negative cycles and even there it is only needed for the output, see Section **??**. We can also get rid of $+\infty$ by noting that $parent(v) = \perp$ iff $d[v] = +\infty$, i.e., when $parent(v) = \perp$, we assume $d[v] = +\infty$ and ignore the number stored in $d[v]$.

A refined implementation of the Bellman-Ford algorithm [178, 127] explicitly maintains a current approximation T of the shortest path tree. Nodes still to be scanned in the current iteration of the main loop are stored in a set Q. Consider the relaxation of an edge $e = (u, v)$ that reduces $d[v]$. All descendants of v in T will subsequently receive a new d-value. Hence, there is no reason to scan these nodes with their current d-values and one may remove them from Q and T. Furthermore, negative cycles can be detected by checking whether v is an ancestor of u in T.

C++: LEDA has special priority queue classes $node\_pq$ that places queue items in graph nodes. Both LEDA and the Boost graph library [28] have implementations of the algorithms of Dijkstra and Bellman-Ford and the algorithms for acyclic graphs and the all-pairs problem. There is a graph iterator based on Dijkstra's algorithm that allows more flexible control of the search process. For example, you can use it to search until a given set of target nodes has been found. LEDA also provides a function that verifies the correctness of distance functions (see Exercise 177).

Java: JDSL [77] provides Dijkstra's algorithm for integer edge costs. It allows similarly detailed control over the search as the graph iterators of LEDA and Boost.

10.9 Historical Notes and Further Findings

Dijkstra [57], Bellman [16] and Ford [63] found their algorithms in the fifties. The original version of Dijkstra's algorithm had running time $O(m + n^2)$ and there is a long history of improvements. Most improvements result from better data structures for priority queues. We discussed binary heaps [195], Fibonacci heaps [67], bucket heaps [54], and radix heaps [7]. Experimental comparisons can be found in [41, 127]. For integer keys, radix heaps are not the end of the story. The best theoretical result is $\mathcal{O}(m + n \log\log n)$ time [183]. Interestingly, for *undirected* graphs, linear time can be achieved [180]. The latter algorithm still settles nodes one after the other but not in the same order as Dijkstra's algorithm. [ps: removed duplicate mention of the ⟹ linear time results] [ps: moved Noshita citation to the place of the average ⟹ case theorem.]

Integrality of edge costs is of use also when negative edges costs are allowed. If all edge costs are integers greater than $-N$, a *scaling algorithm* achieves time $\mathcal{O}(m\sqrt{n}\log N)$ [76].

In Section 10.7 we outlined a small number of speedup techniques for route planning. Many other techniques exist. In particular, we have not mentioned advanced goal directed techniques, combinations of different techniques, etc. A recent overview can be found in [156]. Theoretical performance guarantees beyond Dijkstra's algorithm are more difficult to achieve. Some work for specialized graph families such as planar graphs, some only give approximations, and some combine both kinds of restrictions, e.g., [**?** 184, 181]. [ps: Ãijberarbeitet. Aber vermutlich ⟹ hat Kurt noch konkretere Wuensche???]

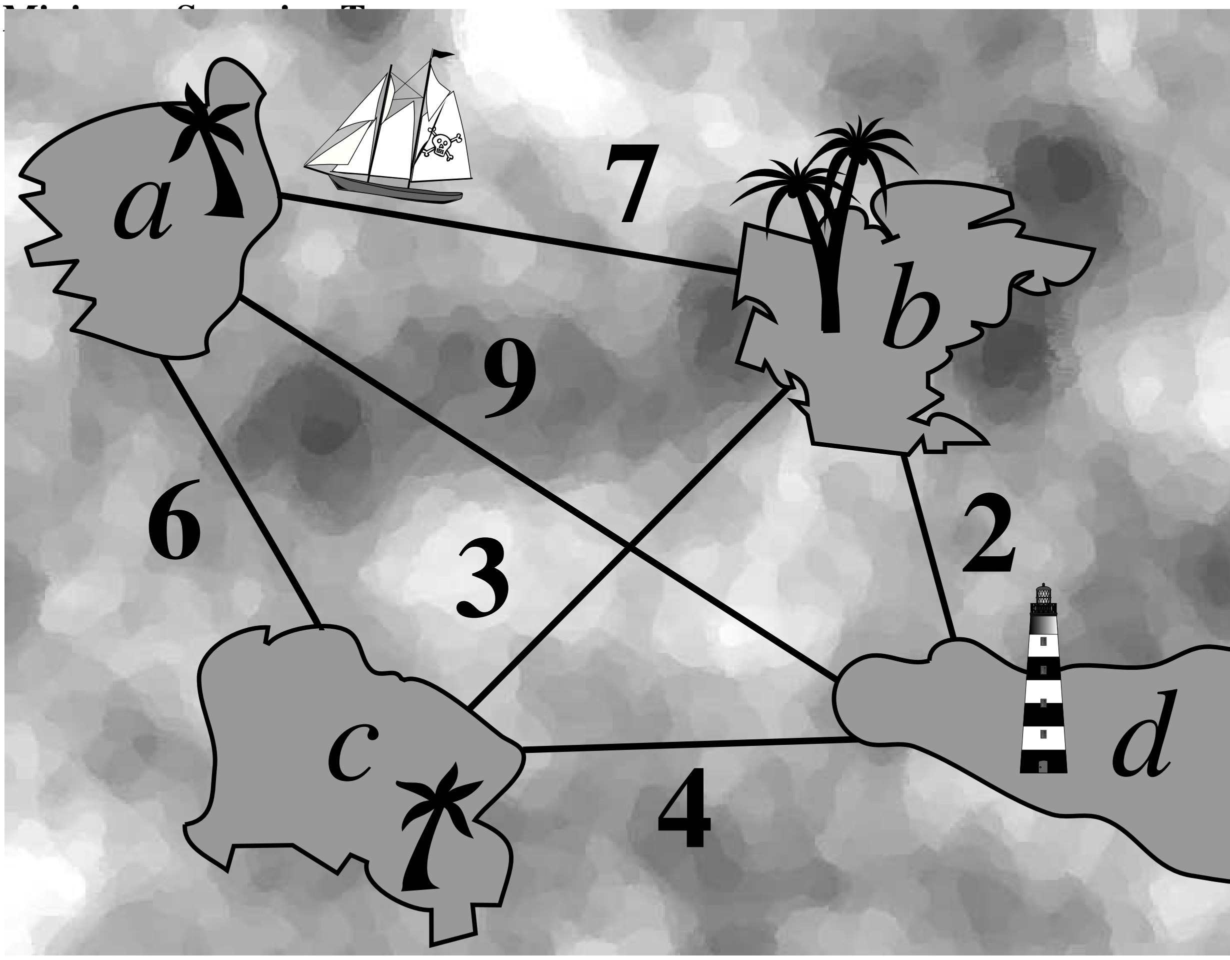
A generalization of the shortest path problem considers several cost functions at once. For example, your grandfather might want to know the fastest route for visiting you but he only wants routes where he does not need to refuel his car or you may want to know the fastest route subject to the condition that road toll does not exceed a certain limit. Constrained shortest path problems are discussed in [84, 130].

Shortest paths can also be computed in geometric settings. In particular, there is an interesting connection to optics. Different materials can have a different refractive index which is related to the speed of light in this medium. Astonishingly, the laws of optics dictate that a ray of light always travels along a shortest path.

Exercise 191. An ordered semi-group is a set S together with an associative and commutative operation $+$, a neutral element 0, and a linear ordering $\leq$ such that for all x, y, and z: $x \leq y$ implies $x + z \leq y + z$. Which of the algorithms of this chapter work for ordered semi-groups? Which work under the additional assumption that $0 \leq x$ for all x?

11

Minimum Spanning Trees



The atoll Taka-Tuka-Land in the South Seas asks you for help. They want to connect their islands by ferry lines. Since money is scarce, the total cost of the opened connections should be minimal. It should be possible to travel between any two islands but direct connections are not necessary. You are given a list of possible connections together with their estimated cost. Which connections should be opened?

More generally, we want to solve the following problem: Consider a connected undirected graph $G = (V, E)$ with real edge costs $c : E \to \mathbb{R}_+$. A *minimum span-*

ning tree (MST) of G is defined by a set $T \subseteq E$ of edges such that the graph (V,T) is a tree $c(T) := \sum_{e \in T} c(e)$ is minimized. In our example, the nodes are islands, the edges are possible ferry connections, and the costs are the costs of opening a connection. Throughout this chapter, G denotes an undirected connected graph.

Minimum spanning trees (MSTs) are perhaps the simplest variant of an important family of problems known as *network design problems*. Because MSTs are such a simple concept, they also show up in many seemingly unrelated problems such as clustering, finding paths that minimize the maximum edge cost used, or finding approximations for harder problems. Section 11.9 has more on that. An equally good reason to discuss MSTs in an algorithms text book is that there are simple, elegant, and fast algorithms to find them. We will derive two simple properties of MSTs in Section 11.1. They form the basis of most MST algorithms. The Jarník-Prim algorithm grows an MST starting from a single node and will be discussed in Section 11.2. Kruskal's algorithm grows many trees in unrelated parts of the graph and merges them into larger and larger trees. It will be discussed in Section 11.3. An efficient implementation of the algorithm requires a data structure for maintaining partitions of a set of elements under two operations: "determine whether two elements are in the same subset" and "join two subsets". We will discuss the so-called union-find data structure in Section 11.4. It has many applications besides the construction of minimum spanning trees.

Exercise 192. If the input graph is not connected, we may ask for a *minimum spanning forest* — a set of edges that defines an MST for each connected component of G. Develop an efficient way to find minimum spanning forests using a single call of a minimum spanning tree routine. Do not find connected components first. Hint: insert $n - 1$ additional edges.

Exercise 193 (Spanning Sets). A set T of edges spans a connected graph G if (V,T) is connected. Is a minimum cost spanning set of edges necessarily a tree? Is it a tree if all edge costs are positive?

Exercise 194. Reduce the problem of finding *maximum* cost spanning trees to the minimum spanning tree problem.

11.1 Cut and Cycle Properties

We prove two simple Lemmas which allow one to add edges to an MST and to exclude edges from an MST. edges from consideration for an MST. We need the concept of a cut in a graph. A *cut* in a connected graph is a subset E' of edges such that $G \setminus E'$ is not connected. Here, $G \setminus E'$ is a short-hand for $(V, E \setminus E')$. If S is a set of nodes with $\emptyset \neq S \neq V$, the set of edges with exactly one endpoint in S forms a cut. Figure 11.1 illustrates the proofs of the following Lemmas.

Lemma 31 (Cut Property). *Let E' be a cut and let e be a minimal cost edge in E'. Then there is an MST T of G that contains e. Moreover, if T' is a set of edges that is*

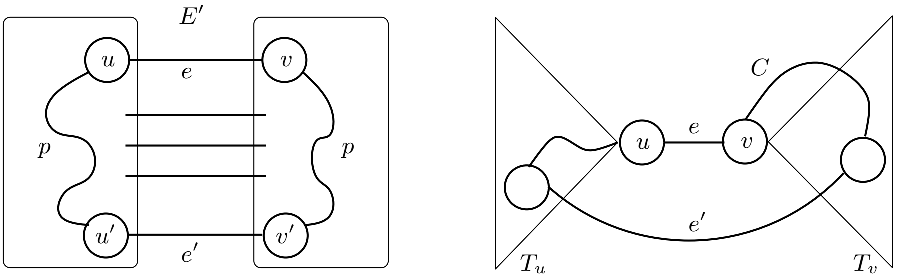


Fig. 11.1. Cut and Cycle Properties. The figure on the left illustrates the proof of the cut property. e is an edge of minimum cost in the cut E' and p is a path in the MST connecting the endpoints of e. p must contain an edge in E'. The figure on the right illustrates the proof of the cycle property. C is a cycle in G, e is an edge of C of maximal weight and T is an MST containing e. T_u and T_v are the components of $T \setminus e$ and e' is an edge in C connecting T_u and T_v.

contained in some MST and T' contains no edge in E' then $T' \cup \{e\}$ is also contained in some MST.

Proof. We prove the second claim. The first claim follows by setting $T' = \emptyset$. Consider any MST T of G with $T' \subseteq T$. Let u and v be the endpoints of e. Since T is a spanning tree, it contains a path from u to v, say p. Since E' is a cut and u and v are separated by it, p must contain an edge in E', say e'. Now, $T'' := (T \setminus e') \cup e$ is also a spanning tree, because removal of e' splits T into two subtrees which are then joined together by e. Since $c(e) \leq c(e')$, we have $c(T'') \leq c(T)$, and hence, T'' is also an MST.

Lemma 32 (Cycle Property). *Consider any cycle $C \subseteq E$ and an edge $e \in C$ with maximal cost among all edges of C. Then any MST of $G' = (V, E \setminus \{e\})$ is also an MST of G.*

Proof. Consider any MST T of G. Suppose T contains $e = (u, v)$. Edge e splits T into two subtrees T_u and T_v. There must be another edge $e' = (u', v')$ from C such that $u' \in T_u$ and $v' \in T_v$. $T' := (T \setminus \{e\}) \cup \{e'\}$ is a spanning tree which does not contain e. Since $c(e') \leq c(e)$, T' is also an MST.

The cut property gives rise to a simple greedy algorithm for finding a minimum spanning tree: start with an empty set T of edges. While T is not a spanning tree, let E' be a cut not containing any edge in T. Add a minimal cost edge in E' to T.

Different choices of E' lead to different specific algorithms. We discuss two approaches in detail in the following sections and outline a third approach in Section 11.9. Also, we need to explain[ps was:detail] how to find a minimum cost edge ⟸
in the cut.

The cycle property also gives rise to a simple algorithm for finding a minimum spanning tree. Set T to the set of all edges. While T is not a spanning tree, find a

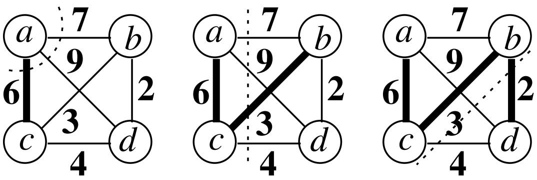


Fig. 11.2. A sequence of cuts (dotted lines) corresponding to an execution of the Jarník-Prim Algorithm with starting node a. The edges (a, c), (c, b) and (b, d) are added to the MST.

```
Function jpMST : Set of Edge
    d = ⟨∞, ..., ∞⟩ : NodeArray[1..n] of $\mathbb{R} \cup \{\infty\}$   // $d[v]$ is the distance of $v$ from the tree
    parent : NodeArray of NodeId                    // parent[$v$] is shortest edge between $S$ and $v$
    $Q$ : NodePQ                                    // uses $d[\cdot]$ as priority
    $Q$.insert($s$) for some arbitrary $s \in V$
    while $Q \neq \emptyset$ do
        $u$ :=$Q$.deleteMin
        $d[u]$ :=0                                  // $d[u] = 0$ encodes $u \in S$
        foreach edge $e = (u, v) \in E$ do
            if $c(e) < d[v]$ then                   // $c(e) < d[v]$ implies $d[v] > 0$ and hence $v \notin S$
                $d[v]$ :=$c(e)$
                parent[$v$] :=$u$
                if $v \in Q$ then $Q$.decreaseKey($v$) else $Q$.insert($v$)
        invariant $\forall v \in Q : d[v] = \min\{c((u, v)) : (u, v) \in E \wedge u \in S\}$
    return $\{(v, parent[v]) : v \in V \setminus \{s\}\}$
```

Fig. 11.3. The Jarník-Prim MST Algorithm. Positive edge costs are assumed.

cycle in T and delete an edge of maximal cost from T. No efficient implementation of this approach is known and we will not discuss it further.

Exercise 195. Show that the MST is uniquely defined if all edge costs are different. Show that in this case the MST does not change if each edge cost is replaced by its rank among all edge costs.

11.2 The Jarník-Prim Algorithm

The Jarník-Prim (JP) algorithm for MSTs is very similar to Dijkstra's algorithm for shortest paths.[1] Starting from an (arbitrary) source node s, the JP algorithm grows a minimum spanning tree by adding one node after the other. At any iteration, S is the set of nodes already added to the tree and the cut E' is the set of edges with

[1] Actually Dijkstra also describes this algorithm in his seminal 1959 paper on shortest paths [57]. Since Prim described the same algorithm two years earlier it is usually named after him. However, the algorithm actually goes back to a 1930 paper by Jarník [96].

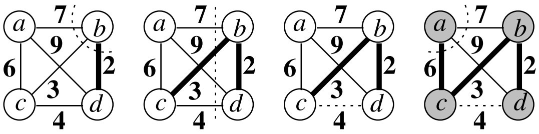


Fig. 11.4. In this example, Kruskal's algorithm first proves that (b, d) and (b, c) are MST edges using the cut property. Then (c, d) is excluded because it is the heaviest edge on the cycle $\langle b, c, d\rangle$, and, finally, (a, b) completes the MST.

exactly one endpoint in S. A minimum cost edge leaving S is added to the tree in every iteration. The main challenge is to find this edge efficiently. To this end, the algorithm maintains the shortest connection between any node $v \in V \setminus S$ to S in a priority queue Q. The smallest element in Q gives the desired edge. When a node is added to S, its incident edges are checked to see whether they yield improved connections to nodes in $V \setminus S$. Figure 11.3 shows the pseudocode for the JP algorithm and Figure 11.2 illustrates an execution. When node u is added to S and an incident edge $e = (u, v)$ is inspected, the algorithm needs to know whether $v \in S$. A bit-vector could be used to encode this information. When all edge costs are positive, we may reuse the d-array to encode this information. For any node v, $d[v] = 0$ encodes $v \in S$ and $d[v] > 0$ encodes $v \notin S$. This small trick does not only save space, but also saves a comparison in the innermost loop. Observe that $c(e) < d[v]$ is only true if $d[v] > 0$, i.e., $v \notin S$, and e is an improved connection for v to S.

The only important difference to Dijkstra's algorithm is that the priority queue stores edge costs rather than path lengths. The analysis of Dijkstra's algorithm carries over to the JP algorithm, i.e., the use of a Fibonacci heap priority queue yields running time $\mathcal{O}(n \log n + m)$.

Exercise 196. Dijkstra's algorithm for shortest paths can use monotone priority queues. Show that monotone priority queues do *not* suffice for the JP algorithm.

***Exercise 197 (Average case analysis of the JP algorithm)** Assume the edge costs $1,\ldots,m$ are randomly assigned to the edges of G. Show that the expected number of *decreaseKey* operations performed by the JP algorithm is then bounded by $\mathcal{O}\big(n \log \frac{m}{n}\big)$. Hint: the analysis is very similar to the average case analysis of Dijkstra's algorithm in Theorem 29.

11.3 Kruskal's Algorithm

The JP algorithm is probably the best general purpose MST algorithm. Nevertheless, we will now present an alternative algorithm, Kruskal's algorithm [113]. It also has its merits. In particular, it does not need a sophisticated graph representation, but already works when the graph is represented by its list of edges. Also for sparse graphs with $m = \mathcal{O}(n)$, its running time is competitive with the JP algorithm.

```
Function kruskalMST(V, E, c) : Set of Edge
    $T := \emptyset$
    invariant $T$ is a subforest of an MST
    foreach $(u, v) \in E$ in ascending order of cost do
        if $u$ and $v$ are in different subtrees of $T$ then
            $T := T \cup \{(u, v)\}$                              // join two subtrees
    return $T$
```

Fig. 11.5. Kruskal's MST algorithm.

The pseudocode given in Figure 11.5 is extremely compact. The algorithm scans over the edges of G in order of increasing cost and maintains a partial MST T; T is empty initially. The algorithm maintains the invariant that T can be extended to an MST. When an edge e is considered, it is either discarded or added to the MST. The decision is made on the basis of the cycle or cut property. The endpoints of e either belong to the same connected component of (V, T) or not. In the former case, $T \cup e$ contains a cycle and e is an edge of maximum cost in this cycle; here it is essential that edges are considered in order of increasing cost. Therefore e can be discarded by the cycle property. In the latter case, e is a minimum cost edge in the cut E' consisting of all edges connecting distinct components of (V, T); again, it is essential that edges are considered in order of increasing cost. We may therefore add e to T by the cut property. The invariant is maintained.

The most interesting algorithmic aspect of Kruskal's algorithm is how to implement the test whether an edge connects to components of (V, T). In the next section we will see that this can be implemented very efficiently so that the main cost factor is sorting the edges. This takes time $\mathcal{O}(m \log m)$ if we use an efficient comparison-based sorting algorithm. The constant factor involved is rather small so that for $m = \mathcal{O}(n)$ we can hope to do better than the $\mathcal{O}(m + n \log n)$ JP algorithm.

Exercise 198 (Streaming MST). Suppose the edges of a graph are presented to you only once (for example over a network connection) and you do not have enough memory to store all of them. The edges do *not* necessarily arrive in sorted order.

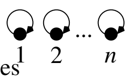
1. Outline an algorithm that nevertheless computes an MST using space $\mathcal{O}(V)$.

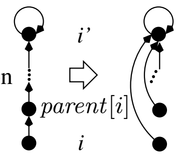
*b) Refine your algorithm to run in time $\mathcal{O}(m \log n)$. Hint: Process batches of $\mathcal{O}(n)$ edges or use the *dynamic tree* data structure by Sleator and Tarjan [172].

11.4 The Union-Find Data Structure

A *partition* of a set M is a collection $M_1, \ldots, M_k$ of subsets of M with the property that the subsets are disjoint and cover M, i.e., $M_i \cap M_j = \emptyset$ for $i \neq j$ and $M = M_1 \cup \cdots \cup M_k$. The subsets M_i are also called the blocks of the partition. For example, in Kruskal's algorithm the forest T partitions V. The blocks of the partition are the connected components of (V, T). Some components may be trivial and consist of a

```
Class UnionFind($n : \mathbb{N}$)                     // Maintain a partition of $1..n$
    parent = $\langle 1, 2, \ldots, n \rangle$ : $Array\ [1..n]$ of $1..n$
    seniority = $\langle 0, \ldots, 0 \rangle$ : $Array\ [1..n]$ of $0..\log n$ // seniority of representatives

Function find($i : 1..n$) : $1..n$
    if $parent[i] = i$ then return $i$
    else $i' :=$find($parent[i]$)                       // path compression
        $parent[i] := i'$
        return $i'$

Procedure link($i, j : 1..n$)
    assert $i$ and $j$ are representatives of different blocks
    if $seniority[i] < seniority[j]$ then $parent[i] := j$
    else
        $parent[j] := i$
        if $seniority[i] = seniority[j]$ then $seniority[i]$++

Procedure union($i, j : 1..n$)
    if $find(i) \neq find(j)$ then $link(find(i), find(j))$
```





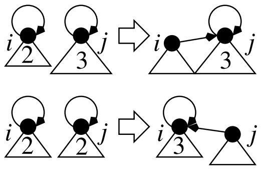


Fig. 11.6. An efficient Union-Find data structure maintaining a partition of the set $\{1, \ldots, n\}$.

single isolated node. Kruskal's algorithms performs two operations on the partition: testing whether two elements are in the same subset (subtree) and joining two subsets into one (inserting an edge into T).

The *union-find data structure* maintains a partition of the set $1..n$ and supports these two operations. Initially, each element is a block of its own. Each block chooses one of its elements as its representative; the choice is made by the data structure and not by the user. The function $find(i)$ returns the representative of the block containing i. Thus, testing whether two elements are in the same block, amounts to comparing their respective representatives. Operation $link(i, j)$ applied to representatives of different blocks joins the blocks.

A simple solution is as follows: each block is represented as a rooted tree[2] with the root being the representative of the block. Each element stores its parent in this tree (array $parent$). We have self-loops at the roots.

The implementation of $find(i)$ is trivial. We follow parent pointers until we encounter a self-loop. The self-loop is at the representative of i. The implementation of $link(i, j)$ is equally simple. We simply make one representative the parent of the other. Then this represenative ceases to be a representative and the other becomes the representative of the combined blocks. What we have said so far yields a correct but inefficient union-find data structure. The $parent$ references could form long chains that are traversed again and again during $find$ operations. In the worst case, each operation may take linear time.

[2] Note that this tree may have a very different structure compared to the corresponding subtree in Kruskal's algorithm.

Exercise 199. Give an example for an n node graph with $\mathcal{O}(n)$ edges where a naive implementation of the union-find data structure without balancing or path compression would lead to quadratic execution time for Kruskal's algorithm.

Therefore, Figure 11.6 makes two optimizations. The first optimization limits the maximal depth of the trees representing blocks. Every representative stores a non-negative integer which we call its *seniority*. Initally, every element is a representative and has seniority zero. When we link two representatives and their seniority is different, we make the representative of smaller seniority a child of the representative of larger seniority. When their seniority is the same, the choice of who becomes parent is arbitrary; however, we increase the seniority of the new root. We refer to the first optimization as *union by seniority*.

Exercise 200. Assume that the second optimization is not used. Show that the seniority of a representative is the height of the tree rooted at it.

Theorem 32. *Union by seniority ensures that the depth of no tree exceeds* $\log n$.

Proof. Without path compression the seniority of a representative is equal to the height of the tree rooted at it. Path compression does not increase heights. It therefore suffices to prove that seniority is bounded by $\log n$. We show that a tree whose root has seniority k contains at least 2^k elements. This is certainly true for $k = 0$. The seniority of a root grows from $k - 1$ to k, when it receives a child of seniority $k - 1$. Thus the root had at least 2^{k-1} descendants before the link operation and it receives a child which also had at least 2^{k-1} descendants. So the root has at least 2^k descendants after the link operation.

The second optimization is called *path compression*. It ensures that a chain of parent references is never traversed twice. Rather, all nodes visited during an operation *find*(i), redirect their parent pointer directly to the representative of i. In Figure 11.6, we have formulated this rule as a recursive procedure. It first traverses the path from i to its represenative and then uses the recursion stack to traverse the path back to i. When the recursion stack is unraveled, the parent pointers are redirected. Alternatively, one may direct the path twice in forward direction. In the first traversal, one finds the representative, and in the second traversal, one redirects the parent pointers.

Exercise 201. Describe a non-recursive implementation of *find*.

Union by seniority and path compression make the union-find data structure "breath-takingly" efficient — the amortized cost of any operation almost constant.

Theorem 33. *The union-find data structure of Figure 11.6 realizes* m *find and* $n - 1$ *link operations in time* $\mathcal{O}(m\alpha_T(m, n))$. *Here*

$$\alpha_T(m, n) = \min\left\{i \geq 1 : A(i, \lceil m/n \rceil) \geq \log n\right\}$$

where

$$\begin{aligned}
A(1,j) &= 2^j && \textit{for } j \geq 1\\
A(i,1) &= A(i-1,2) && \textit{for } i \geq 2\\
A(i,j) &= A(i-1, A(i,j-1)) && \textit{for } i \geq 2 \textit{ and } j \geq 2
\end{aligned}$$

Proof. The proof of this theorem is beyond the scope of this introductory text. We refer the reader to [166] and [175].

You probably find the formulae overwhelming. The function[3] A grows extremely fast. We have $A(1,j) = 2^j$, $A(2,1) = A(1,2) = 2^2 = 4$, $A(2,2) = A(1, A(2,1)) = 2^4 = 16$, $A(2,3) = A(1, A(2,2)) = 2^{16}$, $A(2,4) = 2^{2^{16}}$, $A(2,5) = 2^{2^{2^{16}}}$, $A(3,1) = A(2,2) = 16$, $A(3,2) = A(2, A(3,1)) = A(2,16)$, and so on.

Exercise 202. Estimate $A(5,1)$.

For all practical n, we have $\alpha_T(m,n) \leq 5$, and union-find with union by seniority and path compression essentially guarantees constant amortized cost per operation.

We close this section with an analysis of union-find with path compression but without union by seniority. The analysis illustrates the power of path compression and also gives a glimpse of how Theorem 33 can be proved.

[ps: The following theorem does not give much new insight into the complexity of the combined routine and has a remarkably difficult to understand proof. Drop? Or make easier to understand ?] $\Longleftarrow$

Theorem 34. *The union-find data structure with path compression but without union by seniority processes m find and $n-1$ link operations in time $\mathcal{O}((m+n)\log n)$.*

Proof. [say sth like "It suffices to count parent update ... therefore ..." as an introduction?] We assign a weight to every node of our data structure. The weight $\Longleftarrow$ of a node is the maximal number of descendants of the node (including itself) during the evolution of the data structure. Observe that the weight of a node may increase as long as the node is a representative, has maximal value when the node ceases to be a representative, and may decrease[ps does not understand how the decreas can happen.] due to find operations. We write $w(x)$ for the weight of node x. Weights $\Longleftarrow$ are integers in the range $1..n$. All edges ever existing in our data structure go from nodes of smaller weight to nodes of larger weight.

[ps: there is a barrage of interconnected definitions here. Not so easy to understand.] The span of an edge in our data structure is defined as the weight $\Longleftarrow$ difference of its endpoints. We say that an edge has class i if its span lies in the range $2^i..2^{i+1}-1$. The class of any edge lies between 0 and $\lceil \log n \rceil$ inclusive[ps: is this correct English?]. $\Longleftarrow$

Consider a particular node x. The first edge out of x is created when x ceases to be a representative. [ps does not understand what the next phrase means.]Later $\Longleftarrow$

[3] The usage of the letter A is a reference to the logician Ackermann who first studied a variant of this function in the late 1920s.

edges out of x are created when a find operation passes through the edge $(x, parent(x))$ and this edge is not the last edge traversed by the find. The new edge out of x has a larger span.

[The first two thirds of this proof seems completely unmotivated until, at the very end, things slowly start to make sense. But then we have already losst 99.99??? of the readers? Explain the basic proof strategy at the beginning?] ⟹ We account for the edges out of x as follows. The first edge is charged to the union operation. Consider now any edge $e = (x, y)$ and the find operation which destroys it. Let e have class i. The find operation traverses a path of edges. If e is the last (= topmost) edge of class i traversed by the find, we charge the construction of the new edge out of x to the find operation, otherwise, we charge it to x. Observe ⟹ that in this way,[ps added comma] at most $1 + \lceil \log n \rceil$ edges are charged to any ⟹ find operation[ps: why? This is not obvious to me.]. If the construction of the new edge out of x is charged to x, there is another edge $e' = (x', y')$ following e on the find path. Also, the new edge out of x has a span at least as large as the sum of the spans of e and e' since it goes to an ancestor (not necessarily proper[ps: is ⟹ this good English?]) of y'. Thus the new edge edge out of x has a spanof at least $2^i + 2^i = 2^{i+1}$ and hence is in class $i + 1$ or higher. We conclude that at most one edge in each class is constructed for every node x. Thus the total number of edges constructed is at most $n + (n + m)(1 + \lceil \log n \rceil)$ and the time bound follows.

11.5 Certification of Minimum Spanning Trees

The Jarník-Prim and the Kruskal algorithm for minimum spanning trees are so simple that it is hard to implement them incorrectly[This is a reason why certification is NOT interesting here. What about a more convincing intro? For example by saying that MST algorithms for parallel or external memory are more com- ⟹ plicated and also more likely to suffer hardware errors?]. Of course, both of them use data structures, namely priority queues and union-find, respectively[It is ⟹ not clear to ps why this makes certification interesting]. In this section, we want to discuss certificates for minimum spanning trees. The cut property gives a simple criterion.

Let T be a spanning tree. For any non-tree edge e, let p_e be the path in T connecting the endpoints of e. If for any $e \in E \setminus T$, the cost of e is at least as large at the cost of any edge in p_e, T is a minimum spanning tree. Can this criterion be checked efficiently? A first way of doing it as follows. Select an arbitrary node r and make it the root of T. Orient all edges of T towards the root. For any two nodes u and v, let $lca(u, v)$ be the lowest common ancestor of u and v. Then, for $e = (u, v)$ the path from u to v consists of the path from u to $lca(u, v)$ followed by the path from $lca(u, v)$ to v. We can find the maximum cost edge on this path in time $\mathcal{O}(n)$ and hence can check the cycle property for all edges in time $\mathcal{O}(mn)$. This is quite slow compared to the construction time for MSTs.

We sketch an improvement. Let $T = \{e_1, e_2, \ldots, e_{n-1}\}$ be a minimum spanning tree where the edges are ordered such that $c(e_1) \le c(e_2) \le \ldots \le c(e_{n-1})$. We

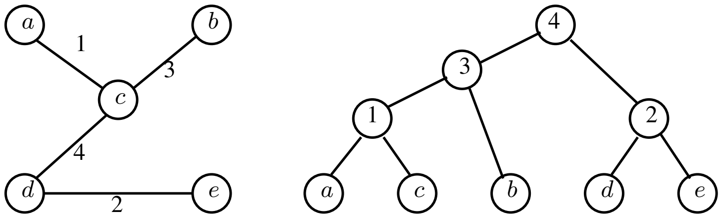


Fig. 11.7. An MST and the corresponding auxiliary tree.

use an auxiliary tree T_A[ps: changed $T_a \to T_A$ everywhere to avoid confusion with node a in the example. OK?] for visualizing the evolution of T as the edges $\Longleftarrow$ of T are added in increasing order of cost: T_A has n leaves, one for each node of G, and $n-1$ internal nodes, one for each edge of T. The internal nodes also represent subsets of nodes. The node for edge e_i represents the connected component of $(V, \{e_1, \dots, e_i\})$ containing e_i. The children of the node for e_i are the connected components of $(V, \{e_1, \dots, e_{i-1}\})$ joined by e_i. Figure 11.7 gives an example. T_a has several useful properties. First, the cost of the edges associated with the internal nodes of any leaf to root path are in non-decreasing order. Second, for any edge $e = (u, v)$, the cost of the edge associated with $lca(u, v)$ is the maximum cost edge on p_e. We therefore only have to check that $c(e)$ is at least $c(lca(u, v))$. Fortunately, there are very fast and compact data structures for the lca-problem [85, 23, 19]. They can be constructed in linear time and find the least common ancestor of any pair of nodes in constant time. With these data structures the verification of spanning trees takes time $O(n + m)$ plus the time to sort the spanning tree edges by weight. Linear time verification algorithms exist. [ps from here on new]These are based on $\Longleftarrow$ sophisticated algorithms that can compute least common ancestors, or minima over arbitrary intervals of an array in constant time [17]. Algorithms for MST verification are also an ingredient of a randomized linear time algorithm outlined in Section 11.9.

11.6 External Memory

The MST problem is one of very few problems on graphs that is known to have an efficient external memory algorithm. We will give a simple and elegant algorithm that exemplifies many interesting techniques that are also useful for other external memory algorithms or for computing MSTs in other models of computation. Our algorithm is a composition of techniques that we have already seen: external sorting, priority queues, and internal union-find. More details can be found in [52].

11.6.1 Semi-External Kruskal

We begin with an easy case. Suppose we have enough internal memory to store the union-find data structure from Section 11.4 for n nodes. This is enough to implement

Kruskal's algorithm in the external memory model. We first sort the edges using the external memory sorting algorithm from Section 5.7. Then we scan the edges in order of increasing weight and process them as described by Kruskal's algorithm. If an edge connects two subtrees, it is an MST edge and can be output; otherwise, it is discarded. External memory graph algorithms that require $\Theta(n)$ internal memory are called *semi-external* algorithms.

Exercise 203 (Streaming Algorithm). Consider a graph with n nodes and m edges. The edges are stored in a file in no particular order. Suppose you have enough internal memory to find an MST for any graph with n nodes and at most $2n$ edges. Explain how to find the MST of the entire graph if you are only allowed to scan the input file once.

11.6.2 Edge Contraction

If the graph has too many nodes for the semi-external algorithm of the preceding section, we can try to reduce the number of nodes. This can be done using *edge contraction*. Suppose, we know that $e = (u, v)$ is an MST edge, e.g., because e is the least weight edge incident to v. We add e and somehow need to remember that u and v are already connected in the MST under construction. Above, we used the union-find data structure to record this fact; now we use edge constraction to encode the information into the graph itself. We identify u and v and replace them by a single node. For simplicity, we call this node again u. In other words, we delete v and *relink* all edges incident to v to u, i.e., any edge (v, w) now becomes edge (u, w). Figure 11.8 gives an example. In order to keep track of the origin of relinked edges, we associate an additional attribute with each edge that indicates its *original* endpoints. With this additional information, an MST of the contracted graph is easily translated back to the original graph. We simply replace each edge by its original.

We now have a blue print for an external MST algorithm: repeatedly find MST edges and contract them. Once the number of nodes is small enough, switch to a semi-external algorithm. The following section gives a particularly simple implementation of this idea.

11.6.3 Sibeyn's Algorithm

Suppose $V = 1..n$. Consider the following simple strategy for reducing the number of nodes from n to n' [52]:

```
**for** $v := 1$ **to** $n - n'$ **do**
    *find the lightest edge $(u, v)$ incident to $v$ and contract it*
```

Figure 11.8 gives an example with $n = 4$ and $n' = 2$. The strategy looks deceivingly simple. We need to discuss how we find the cheapest edge incident to v and how we relink the other edges incident to v, i.e., how we inform the neighbors of v that additional edges become incident to them. We can use a priority queue for both purposes. For each edge, $e = (u, v)$, we store the item

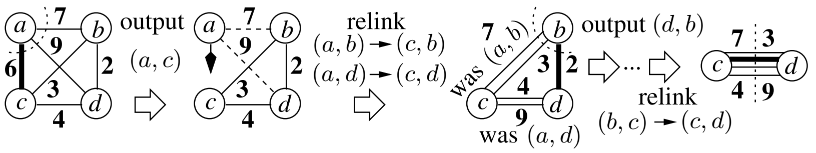


Fig. 11.8. An execution of Sibeyn's algorithm with $n' = 2$. The edge $(c, a, 6)$ is the cheapest edge incident to a. We add it to the MST and merge a into c. The edge $(a, b, 7)$ becomes an edge $(c, b, 7)$ and $(a, d, 9)$ becomes $(c, d, 9)$. In the new graph, $(d, b, 2)$ is the cheapest edge incident to b. We add it to the spanning tree and merge b into d. The edges $(b, c, 3)$ and $(b, c, 7)$ become $(d, c, 3)$ and $(d, c, 7)$, respectively. The resulting graph has two nodes that are connected by four parallel edges of weight 3, 4, 7, and 9, respectively.

```
Function sibeynMST(V, E, c) : Set of Edge
    let $\pi$ be a random permutation of $1..n$
    Q: priority queue                         // Order: min node, then min edge weight
    foreach $e = (u, v) \in E$ do
        Q.insert($\min\{\pi(u), \pi(v)\}, \max\{\pi(u), \pi(v)\}, c(e), u, v)$)
    current := 0                              // we are just before processing node 1
    loop
        $(u, v, c, u_0, v_0)$ :=min Q                                      // next edge
        if current $\neq u$ then                                           // new node
            if $u = n - n' + 1$ then break loop              // node reduction completed
            Q.deleteMin
            output $(u_0, v_0)$                  // the original endpoints define an MST edge
            (current, relinkTo) :=$(u, v)$       // prepare for relinking remaining $u$-edges
        else if $v \neq$ relinkTo then
            Q.insert(($\min\{v$, relinkTo$\}, \max\{v$, relinkTo$\}, c, u_0, v_0$))      // relink
    S := sort(Q)                                       // sort by increasing edge weight
    apply semi-external Kruskal to S
```

Fig. 11.9. Sibeyns's MST algorithm.

$$(\min(u, v), \max(u, v), \text{weight of } e, \text{origin of } e)$$

in the priority queue. The ordering is lexicographic by first and third components, i.e., edges are ordered according to their lower number endpoint and for equal lower numbered endpoint according to weight. The algorithm operates in phases. In each phase, we select all edges incident to the *current* node. The lightest edge (= first edge delivered by the queue), say $(\mathit{current}, \mathit{relinkTo})$, is added to the MST and all others are relinked. In order to relink an edge $(\mathit{current}, z, c, u_0, v_0)$ with $z \neq \mathit{RelinkTo}$, we add $(\min(z, \mathit{RelinkTo}), \max(z, \mathit{RelinkTo}), c, u_0, v_0)$ to the queue.

Figure 11.9 gives the details. For reasons that will become clear in the analysis, we randomly renumber the nodes before starting the algorithm, i.e., we chose a random permutation of the integers 1 to n and rename any node v as $\pi(v)$. For any edge $e = (u, v)$ we store $(\min\{\pi(u), \pi(v)\}, \max\{\pi(u), \pi(v)\}, c(e), u, v))$ in the queue.

$\Longrightarrow$ [removed repetitive sentence] The main loop stops when the number of nodes is reduced to n'. We complete the construction of the MST by sorting the remaining edges and then running the semi-external Kruskal algorithm on them.

Theorem 35. *The expected number of I/O steps required by algorithm* $\mathit{sibeynMST}$ *is* $\mathcal{O}(\mathrm{sort}(m \ln(n/n')))$ *where* sort *denotes the I/O complexity of sorting.*

Proof. From Section 6.3 we know that an external memory priority queue can execute K queue operations using $\mathcal{O}(\mathrm{sort}(K))$ I/Os. Also, the semi-external Kruskal at the end requires $\mathcal{O}(\mathrm{sort}(m))$ I/Os. Hence, it suffices, to count the number of operations in the reduction phases. Besides the m insertions during initialization, the number of queue operations is proportional to the sum of the degrees of the encountered nodes. Let the random variable X_i denote the degree of node i when
$\Longrightarrow$ it is processed. [Umformuliert um Schachtelsatz zu entschÃďrfen:] Since the nodes are processed in random order, we can use linearity of expectation to evaluate $\mathrm{E}[\sum_{1\le i\le n-n'} X_i] = \sum_{1\le i\le n-n'} \mathrm{E}[X_i]$. The number of edges in the contracted graph is at most m so that the average degree of a graph $n-i+1$ remaining nodes is at most $2m/(n-i+1)$. We get:

$$\begin{aligned}
\mathrm{E}[\sum_{1\le i\le n-n'} X_i] &= \sum_{1\le i\le n-n'} \mathrm{E}[X_i] \le \sum_{1\le i\le n-n'} \frac{2m}{n-i+1} \\
&= 2m\left(\sum_{1\le i\le n} \frac{1}{i} - \sum_{1\le i\le n'} \frac{1}{i}\right) = 2m(H_n - H_{n'}) \\
&= 2m(\ln n - \ln n') + \mathcal{O}(1) = 2m \ln \frac{n}{n'} + \mathcal{O}(1)\ ,
\end{aligned}$$

where $H_n := \sum_{1\le i\le n} 1/i = \ln n + \Theta(1)$ is the n-th harmonic number (see Equation (A.12)).

Note that we could do without switching to semi-external Kruskal. However then the logarithmic factor in the I/O complexity would become $\ln n$ rather than $\ln(n/n')$ and the practical performance would be much worse. Observe that $n' = \Theta(M)$ is a large number, say 10^8. For $n = 10^{12}$, $\ln n$ is three times $\ln(n/n')$.

Exercise 204. For any n give a graph with n nodes and $\mathcal{O}(n)$ edges where Sibeyn's algorithm *without random renumbering* would need $\Omega\left(n^2\right)$ relink operations.

11.7 Applications

The MST problem is useful in attacking many other graph problems. We will discuss the Steiner tree problem and the Traveling Salesman problem.

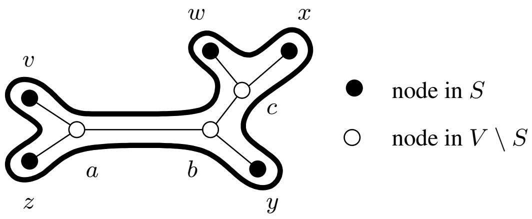


Fig. 11.10. Once around the tree: We have $S = \{v, w, z, y, z\}$ and the minimum Steiner tree is shown. The Steiner tree also involves the nodes a, b and c in $V \setminus S$. Walking once around the tree gives rise to the closed path $\langle v, a, b, c, w, c, x, c, b, y, b, a, z, a, v \rangle$. It maps into the closed path $\langle v, w, x, y, z, v \rangle$ in the auxiliary graph.

11.7.1 The Steiner Tree Problem

We are given a non-negatively weighted undirected graph $G = (V, E)$ and a set S of nodes. The goal is to find a minimum cost subset T of the edges that connects the nodes in S. Such a T is called a minimum Steiner tree. It is a tree connecting a set U with $S \subseteq U \subseteq V$. The art is to choose U as to minimize the cost of the tree. The minimum spanning tree problem is the special case that S consists of all nodes. The Steiner tree problem arises naturally in our introductory example. Assume that some of the islands in Taka-Tuka-land are unihabitated. The goal is to connect all the inhabitated islands. The optimal solution will in general have some of the uninhabitated islands in the solution.

The Steiner tree problem is NP-complete **??**. We show how to construct a solution which is within a factor two of optimum. We construct an auxiliary complete graph with node set S: for any pair u and v of nodes in S, the cost of the edge (u, v) in the auxiliary graph is their shortest path distance in G. Let T_A be a minimum spanning tree of the auxiliary graph. We obtain a Steiner tree of G by replacing every edge of T_A[ps was: T. Ab hier leicht umformuliert] by the path it represents in G. In the $\Longleftarrow$ resulting subgraph of G we delete edges from cycles until it the remaining subgraph is cycle-free. The cost of the resulting Steiner tree is at most the cost of T_A.

Theorem 36. *The algorithm above constructs a Steiner tree which is at most twice the cost of an optimum Steiner tree.*

Proof. The algorithm constructs a Steiner tree of cost at most $c(T_A)$. It therefore suffices to show $c(T_A) \leq 2c(T_{\mathrm{opt}})$, where T_{opt} is a minimum Steiner tree for S in G. To this end, it suffices to show that the auxiliary graph has a spanning tree of cost $2c(T_{\mathrm{opt}})$. Figure 11.10 indicates how to construct such a spanning tree. "Walking once around the Steiner tree" defines a closed path in G of cost $2c(T_{\mathrm{opt}})$; observe that every edge in T_{opt} occurs exactly twice in this path. Deleting the nodes outside S in this path gives us a closed path in the auxiliary graph. The cost of this path is at most $2c(T_{\mathrm{opt}})$, because edge costs in the auxilary graph are shortest path distances in G. The closed path in the auxiliary graph spans S and therefore the auxiliary graph has a spanning tree of cost at most $2c(T_{\mathrm{opt}})$.

Exercise 205. Improve the bound to $2(1 - 1/|S|)$ times the optimum.

The algorithm can be implemented to run in time $\mathcal{O}(m + n \log n)$ [122]. Algorithms with better approximation ratio exist [153].

Exercise 206. Outline an implementation of the algorithm above and analyse its running time.

11.7.2 Traveling Salesman Tours

[ps: inserted sentence]Here is one of most intensively studied optimization problems [1, 114, 11]: Given an undirected complete [ps removed: edge-weighted (abschreckend)] graph on node set V with edge weights $c(e)$, the goal is to find the minimum weight simple cycle [was:closed path] passing through all nodes. This is the path a traveling salesman would want to take whose goal is it to visit all nodes of the graph. We assume for this section that the edge weights satisfy the triangle inequality, i.e., $c(u,v) + c(v,w) \geq c(u,w)$ for all nodes u, v, and w. Then there is always an optimal round-trip which visits no node twice (because leaving it out, would not increase the cost).

Theorem 37. *Let C_{opt} and C_{MST} be the cost of an optimum tour and a minimum spanning tree, respectively. Then*

$$C_{\text{MST}} \leq C_{\text{opt}} \leq 2C_{\text{MST}} .$$

Proof. Let C be an optimal tour. Deleting any edge from C yields a spanning tree. Thus $C_{\text{MST}} \leq C_{\text{opt}}$. Conversely, let T be a minimum spanning tree. Walking once around the tree as shown in Figure 11.10 gives us a cycle[ps was: closed path] of cost at most $2C_{\text{MST}}$ passing through all nodes. It may visit nodes several times. Deleting an extra visit to a node does not increase cost due to the triangle inequality.

In the remainder of this section, we will briefly outline a technique for improving the lower bound of Theorem 37. We need two additional concepts: 2-tree and potential function. A minimum 2-tree consists of the two cheapest edges incident to node 1 and a minimum spanning tree of $G \setminus 1$[ps: define this notation somewhere? Reformulate to avoid it?]. Since deleting the two edges incident to node 1 from a tour C yields a spanning tree of $G \setminus 1$, we have $C_2 \leq C_{\text{opt}}$, where C_2 is the minimum cost of a 2-tree. [ps: refer to definition in SSSP chapter? shorter here? forward ref there?]A potential function is any real-valued function π defined on the nodes of G. Any potential function gives rise to a modified cost function c_π by defining

$$c_\pi(u,v) = c(u,v) + \pi(v) + \pi(u)$$

for any pair u and v of nodes. For any tour C, the cost under c and c_π differ by $2S_\pi := 2\sum_v \pi(v)$ since a tour uses exactly two edges incident to any node. Let T_π be a minimum 2-tree with respect to c_π. Then

$$c_\pi(T_\pi) \leq c_\pi(C_{\text{opt}}) = c(C_{\text{opt}}) + 2S_\pi$$

and hence

$$c(C_{\text{opt}}) \geq \max_\pi \left(c_\pi(T_\pi) - 2S_\pi\right) \ .$$

This lower bound is known as the Held-Karp lower bound [87, 88]. The maximum is over all potential functions π. It is hard to compute the lower bound exactly. However, there are fast iterative algorithms for approximating it. The idea is as follows and we refer the reader to the original papers for details. Assume we have a potential function π and the optimal 2-tree T_π with respect to it. If all nodes of T_π have degree two, we have a Traveling Salesman tour and stop. Otherwise, we make the edges incident to nodes of degree larger than two a bit more expensive and the edges incident to nodes of degree one a bit cheaper. This can be done by modifiying the potential function as follows. We define a new potential function π' by

$$\pi'(v) = \pi(v) + \epsilon \cdot (\deg(v, T_\pi) - 2)$$

where ϵ is a parameter which goes to zero with the iteration number and $\deg(v, T_\pi)$ is the degree of v in T_π. We next compute an optimum 2-tree with respect to π' and hope that it will yield a better lower bound.

11.8 Implementation Notes

The minimum spanning tree algorithms discussed in this chapter are so fast that running time is usually dominated by the time to generate the graphs and appropriate representations. If an adjacency array representation of undirected graphs as described in Section 8.2 is used, then the JP algorithm works well for all m and n in particular if pairing heaps [135] are used for the priority queue. Kruskal's algorithm may be faster for sparse graphs, in particular, if only a list or array of edges is available or if we know how to sort the edges very efficiently.

The union-find data structure can be implemented more space efficiently by exploiting the fact that only representatives need a seniority whereas only non-representatives need a parent. We can therefore omit the array *seniority* in Figure 11.5. Instead, a root of seniority g stores the value $n + 1 + g$ in *parent*. Thus, instead of two arrays, only one array with values in the range $1..n + 1 + \lceil \log n \rceil$ is needed. This is particularly useful for the semi-external algorithm.

C++: LEDA [115] uses Kruskal's algorithm for computing minimum spanning trees. The union-find data structure is called *partition* in LEDA. The Boost graph library [28] gives the choice between Kruskal's algorithm and the JP algorithm. Boost offers no public access to the union-find data structure.

Java: JDSL [77] uses the JP algorithm.

11.9 Historical Notes and Further Findings

The oldest MST algorithm is based on the cut property and uses edge contractions. *Boruvka's algorithm* [29, 140] goes back to 1926 and hence represents one of the oldest graph algorithms. The algorithm operates in phases and identifies many MST edges in each *phase*. In a phase, each node identifies the lightest incident edge. These edges are added to the MST (here it is assumed that edge costs are pairwise distinct) and then contracted. Each phase can be implemented to run in time $\mathcal{O}(m)$. Since a phase at least halves the number of remaining nodes, only a single node is left after $\mathcal{O}(\log n)$ phases and hence the total running time is $\mathcal{O}(m \log n)$. Boruvka's algorithm is not often used because it is somewhat complicated to implement. It is nevertheless important as a basis for parallel MST algorithms.

There is a randomized linear time MST algorithm that uses phases of Boruvka's algorithm to reduce the number of nodes [102, 108]. The second ingredient of this algorithm reduces the number of edges to about $2n$: sample $\mathcal{O}(m/2)$ edges randomly; find an MST T' of the sample; remove edges $e \in E$ that are the heaviest edge on a cycle in $e \cup T'$. The last step is rather difficult to implement efficiently. But at least for rather dense graphs this approach can yield a practical improvement [105]. The linear time algorithm can also be parallelized [83]. An adaptation to the external memory model [2] saves a factor $\ln(n/n')$ in the asymptotic I/O complexity compared to Sibeyn's algorithm but is impractical for currently interesting n due to its much larger constant factor in the $\mathcal{O}$-notation.

The theoretically best known *deterministic* MST algorithm [36, 147] has the interesting property that it has optimal worst case complexity although it is not exactly known what this complexity is. Hence, if you come tomorrow with a completely different deterministic MST algorithm and prove that your algorithm runs in linear time, then we know that the old algorithm also runs in linear time.

Minimum spanning trees define a single path between any pair of nodes. Interestingly, this path is a *bottleneck shortest path* [8, Application 13.3], i.e., it minimizes the maximum edge cost for all paths connecting the nodes in the original graph. Hence, finding an MST amounts to solving the all-pairs bottleneck shortest path problem in time much less than for solving the all-pairs shortest path problem.

A related and even more frequently used application is clustering based on the MST [8, Application 13.5]: by dropping $k - 1$ edges from the MST it can be split into k subtrees. Nodes in a subtree T' are far away from the other nodes in the sense that all paths to nodes in other subtrees use edges that are at least as heavy as the edges used to cut T' out of the MST.

Many applications lead to MST problems on complete graphs. Frequently, these graphs have a compact description, e.g., if the nodes represent points in the plane and edge costs are Euclidian distances (so-called Euclidean minimum spanning trees). In these situations, it is an important concern whether one can rule out most of the edges as too heavy without actually looking at them. This is the case for Euclidean MSTs. It can be shown that Euclidean MSTs are contained in the so-called Delaunay triangulation [47] of the point set. It has linear size and and can be computed in time

$\mathcal{O}(n \log n)$. This leads to an algorithm of the same time complexity for Euclidean MSTs.

We discussed the application of MSTs to the Steiner tree and the Traveling Salesman problem. We refer the reader to the books [8, 11, 114, 112, 188][added ref to Aplegate et al. 2006. Does this supersede Lawler et al.? In this case remove ref here and above.] for more information about these and related problems. ⟸

12

Generic Approaches to Optimization

A smuggler in the mountainous region of Profitania has n items in his cellar. If he sells item i across the border, he makes profit p_i. However, the smuggler's trade union only allows him to carry knapsacks with maximum weight M. If item i has weight w_i, what items should he pack into the knapsack to maximize the profit in his next trip?

This problem, usually called the *knapsack problem*, has many other applications. The books [118, 106] describe many. For example, an investment banker might have an amount M of capital to invest and a set of possible investments each with an expected profit p_i for an investment w_i. In this chapter, we use the knapsack problem as a model problem to illustrate several generic approaches to optimization. These approaches are quite flexible and can be adapted to complicated situations that are ubiquitous in practical applications. In the previous chapters we considered very efficient specific solutions for frequently occurring simple problems such as finding shortest paths or minimum spanning trees. Now we look at generic solution methods that work for a much larger range of applications. Of course, the generic methods usually do not obtain the same efficiency as specific solutions. But, they save development time.

Formally, an optimization problem can be described by a set $\mathcal{U}$ of potential solutions, a set $\mathcal{L}$ of *feasible* solutions, and an *objective function* $f : \mathcal{L} \to \mathbb{R}$. In a *maximization* problem, we are looking for a feasible solution $x^* \in \mathcal{L}$ that maximizes the objective value among all feasible solutions. In a *minimization* problem, we look for a solution minimizing the objective value. In an *existence problem*, f is arbitrary and the question is whether the set of feasible solutions is non-empty.

For example, in the case of the knapsack problem with n items, a potential solution is simply a vector $x = (x_1, \ldots, x_n)$ with $x_i \in \{0, 1\}$. Here $x_i = 1$ indicates that "element i is put into the knapsack" and $x_i = 0$ encodes that "element i is left out". Thus $\mathcal{U} = \{0, 1\}^n$. The profits and weights are specified by vectors $p = (p_1, \ldots, p_n)$ and $w = (w_1, \ldots, w_n)$. A potential solution x is feasible if its weight does not exceed the capacity of the knapsack, i.e., $\sum_{1 \leq i \leq n} w_i x_i \leq M$. The dot-product $w \cdot x$

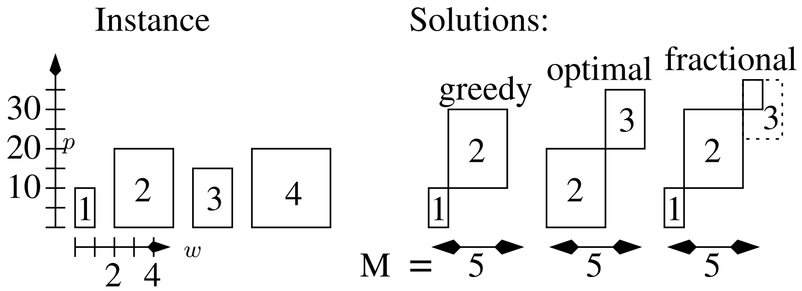


Fig. 12.1. The left part shows a knapsack instance with $p = (10, 20, 15, 20)$, $w = (1, 3, 2, 4)$, and $M = 5$. The items are indicated as rectangles whose width and height correspond to weight and profit, respectively. The right part shows three solutions: the one computed by the greedy algorithm from Section 12.2, an optimal solution computed by the dynamic programming algorithm from Section 12.3, and the solution of the linear relaxation (Section 12.1.1). The optimal solution has weight 5 and profit 35.

is a convenient short-hand for $\sum_{1 \le i \le n} w_i x_i$. Then $\mathcal{L} = \{x \in \mathcal{U} : w \cdot x \le M\}$ is the set of feasible solutions and $f(x) = p \cdot x$ is the objective function.

The distinction between minimization and maximization problems is not essential because setting $f := -f$ converts a maximization problem into a minimization problem and vice versa. We will use maximization as our default simply because our model problem is more naturally viewed as a maximization problem.[1]

We will present seven generic approaches. We start out with black box solvers that can be applied to any problem that can be formulated in the problem specification language of the solver. Then the only task of the user is to formulate the given problem in the language of the black box solver. Section 12.1 introduces this approach using *linear programming* and *integer linear programming* as examples. The *greedy approach* that we have already seen in Section 11 is reviewed in Section 12.2. The *dynamic programming* approach discussed in Section 12.3 is a more flexible way to construct solutions. We can also systematically explore the entire set of potential solutions as described in Section 12.4. *Constraint programming* and *SAT-solvers* are special cases of *systematic search*. Finally we discuss two very flexible approaches to explore only a subset of the solution space. *Local search*, discussed in Section 12.5, modifies a single solution until it has the desired quality. Evolutionary algorithms, explained in Section 12.6, simulate a population of solution candidates.

12.1 Linear Programming — A Black Box Solver

The easiest way to solve an optimization problem is to write down a specification of the space of feasible solutions and of the objective function and then use an existing software package to find an optimal solution. Of course, the question is for what kind

[1] Be aware that most of the literature uses minimization as its default.

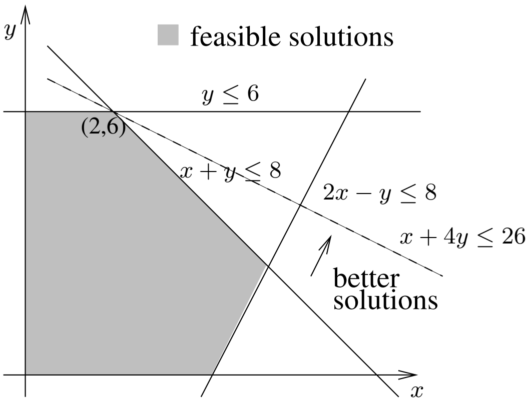


Fig. 12.2. A simple two-dimensional linear program in variables x and y with three constraints and the objective “maximize $x + 4y$”. The feasible region is shaded and $(x, y) = (2, 6)$ is the optimal solution. Its objective value is 26. The vertex $(2, 6)$ is optimal because the half-plane $x + 4y \leq 26$ contains the entire feasible region and has $(2, 6)$ in its boundary.

of specifications are general solvers available? Here we introduce a particularly large class of problems for which efficient black box solvers are available.

Definition 2. *A* Linear Program (LP)[2] *with* n variables *and* m constraints *is a maximization problem defined on a vector* $x = (x_1, \ldots, x_n)$ *of real-valued variables. The objective function is a linear function* f *in* x*, i.e.,* $f : \mathbb{R}^n \to \mathbb{R}$ *with* $f(x) = c \cdot x$ *where* $c = (c_1, \ldots, c_n)$ *is the so-called* cost or profit[3]vector. *The variables are constrained by* m *linear constraints of the form* $a_i \cdot x \bowtie_i b_i$ *where* $\bowtie_i \in \{\leq, \geq, =\}$ *and* $a_i = (a_{i1}, \ldots, a_{in}) \in \mathbb{R}^n$ *and* $b_i \in \mathbb{R}$ *for* $i \in 1..m$*. The set of feasible solutions is given by*

$$\mathcal{L} = \{x \in \mathbb{R}^n : \forall i \in 1..m \text{ and } j \in 1..n : x_j \geq 0 \wedge a_i \cdot x \bowtie_i b_i\} \quad .$$

Figure 12.2 shows a simple example. A classical application of linear programming is the so-called *diet problem*. A farmer wants to mix food for his cows. There are n different kinds of food on the market, say, corn, soya, fish meal,.... One kilogram of food j costs c_j Euro. There are m requirements for healthy nutrition, e.g., the cows should get enough calories, proteins, Vitamin C, and so on. One kilogram of food j contains a_{ij} percent of a cow’s daily requirement with respect to requirement i. Then a solution to the following linear program gives a cost optimal diet satisfying the health constraints: let x_j denote the amount (in kilos) of food j used by the farmer. The i-th nutritional requirement is modelled by the inequality

[2] The term “linear program” stems from the 1940s [46] and has nothing to do with the modern meaning of “program” as in “computer program”.

[3] It is common to use the term profit in maximization problems and cost in minimizations problems.

$\sum_j a_{ij}x_j \geq 100$. The cost of the diet is given by $\sum_j c_j x_j$. The goal is to minimize the cost of the diet.

Exercise 207. How do you model supplies that are available only in limited amounts, e.g., food produced by the farmer himself? Also explain how to specify additional constraints such as "no more than 0.01mg Cadmium contamination per cow and day".

Can the knapsack problem be formulated as a linear program? Probably not, the reason being that the items in the knapsack problem must either put fully into the knapsack or left out completely. There is no possibility of adding an item partially. In contrast, it is assumed in the diet problem that any arbitrary amount of any food can be purchased, e.g., 3.7245 kilos and not just 3 kilos or 4 kilos. Integer linear programs, see Section 12.1.1, are the right tool for the knapsack problem.

We next connect linear programming to the problems we have studied in previous chapters of the book. We show how to formulate the single-source shortest path problem with non-negative edge weights as a linear program. Let $G = (V, E)$ be a directed graph, $s \in V$ the source node, and let $c : E \to \mathbb{R}_{\geq 0}$ be the cost function on the edges of G. In our linear program, we have a variable d_v for every vertex of the graph. The intention is that d_v denotes the cost of the shortest path from s to v. Consider

$$\begin{array}{lll} \text{maximize} & \sum_{v \in V} d_v & \\ \text{subject to} & d_s = 0 & \\ & d_w \leq d_v + c(e) & \text{for all } e = (v, w) \in E \end{array}$$

Theorem 38. *Let $G = (V, E)$ be a directed graph, $s \in V$ a designated vertex, and $c : E \to \mathbb{R}_{\geq 0}$ a non-negative cost function. If all vertices of G are reachable from s, the shortest path distances in G are a solution to the linear program above.*

Proof. Let $\mu(s, v)$ be the length of the shortest path from s to v. Then $\mu(s, v) \in \mathbb{R}_{\geq 0}$ since all nodes are reachable from s and hence no vertex can have distance $+\infty$ from s. We observe first that $d_v := \mu(s, v)$ for all v satisfies the constraints of the LP. Indeed, $\mu(s, s) = 0$ and $\mu(s, w) \leq \mu(s, v) + c(e)$ for any edge $e = (v, w)$.

We next show that if $(d_v)_{v \in V}$ satisfies all constraints of the LP above, then $d_v \leq \mu(s, v)$ for all v. Consider any v, and let $s = v_0, v_1, \ldots, v_k = v$ be a shortest path from s to v. Then $\mu(s, v) = \sum_{0 \leq i < k} c(v_i, v_{i+1})$. We show $d_{v_j} \leq \sum_{0 \leq i < j} c(v_i, v_{i+1})$ by induction on j. For $j = 0$, this follows from $d_s = 0$ by the first constraint. For $j > 0$, we have

$$d_{v_j} \leq d_{v_{j-1}} + c(v_{j-1}, v_j) \leq \sum_{0 \leq i < j-1} c(v_i, v_{i+1}) + c(v_{j-1}, v_j) = \sum_{0 \leq i < j} c(v_i, v_{i+1}) \,,$$

where the first inequality follows from the second set of constraints of the LP and the second inequality comes from the induction hypothesis.

We have now shown that $(\mu(s,v))_{v\in V}$ is a feasible solution and that $d_v \leq \mu(s,v)$ for all v for any feasible solution $(d_v)_{v\in V}$. Since the objective of the LP is to maximize the sum of the d_v, we must have $d_v = \mu(s,v)$ for all v in the optimal solution to the LP.

Exercise 208. Where does the proof above fail, when not all nodes are reachable from s or when there are negative weights? Does it still work in the absence of negative cycles?

The proof that the LP above actually captures the shortest path problem is nontrivial. When you formulate a problem as an LP, you should always prove that the LP is indeed a correct description of the problem that you are trying to solve.

Exercise 209. Let $G = (V,E)$ be a directed graph and s and t be two nodes. Let $cap : E \to \mathbb{R}_{\geq 0}$ and $c : E \to \mathbb{R}_{\geq 0}$ be non-negative functions on the edges of G. For an edge e, we call $cap(e)$ and $c(e)$ the capacity and cost of e, respectively. A flow is a function $f : E \to \mathbb{R}_{\geq 0}$ with $0 \leq f(e) \leq cap(e)$ for all e and flow conservation at all nodes except s and t, i.e., for all $v \neq s,t$ we have

$$\text{flow into } v = \sum_{e=(u,v)} f(e) = \sum_{e=(v,w)} f(e) = \text{flow out of } v\ .$$

The value of the flow is the net flow out of s, i.e., $\sum_{e=(s,v)} f(e) - \sum_{e=(u,s)} f(e)$. The *maximum flow problem* asks for a flow of maximum value. Show that this problem can be formulated as an LP.

The cost of a flow is $\sum_e f(e)c(e)$. The *minimum cost maximum flow problem* asks for a maximum flow of minimum cost. Show how to formulate this problem as an LP.

Linear programs are so important because they combine expressive power with efficient solution algorithms.

Theorem 39. *Linear programs can be solved in polynomial time [107, 103].*

The worst case running time of the best algorithm known is $O\max m, n^{7/2}L$. In this bound it is assumed that all coefficients c_j, a_{ij}, and b_i are integers with absolute value bounded by 2^L; n and m are the number of variables and constraints, respectively. Fortunately, the worst case rarely arises. Most linear programs can be solved relatively quickly by several procedures. One, the simplex algorithm, is briefly outlined in Section 12.5.1. For now, we should remember two facts: first, many problems can be formulated as linear programs, and second, there are efficient linear program solvers that can be used as black boxes. In fact, although LP solvers are used on a routine basis, very few people in the world know exactly how to implement a highly efficient LP solver.

12.1.1 Integer Linear Programming

The expressive power of linear program grows when some or all of the variables can be designated to be integral. Such variables can then take on only integer values and not arbitrary real values. If all variables are constrained to be integral, the problem formulation is called an *Integer Linear Program (ILP)*. If some, but not all, variables are constrained to be integral, the problem formulation is called a *Mixed Integer Linear Program (MILP)*. For example, our knapsack problem is tantamount to the following 0-1 integer linear program

$$\text{maximize } p \cdot x$$

subject to

$$w \cdot x \leq M, \quad \text{and} \quad x_i \in \{0,1\} \text{ for } i \in 1..n \enspace .$$

A 0-1 integer programming problem is one, where the variables are constrained to the values 0 and 1.

Exercise 210. Explain how to replace any ILP by a 0-1 ILP assuming that you know an upper bound U on the value of any variable in the optimal solution. Hint: replace any variable of the original ILP by a set of $\mathcal{O}(\log U)$ 0-1 variables.

Unfortunately, solving ILPs and MILPs is NP-hard. Indeed, even the knapsack problem is NP-hard. Nevertheless, ILPs can often be solved in practice using linear programming packages. In Section 12.4 we will outline how this is done. When an exact solution would be too time-consuming, linear programming can help to find approximate solutions. The *linear program relaxation* of an ILP is the LP obtained by omitting the integrality constraints for the variables. For example in the knapsack problem we would replace the constraint $x_i \in \{0,1\}$ by the constraint $x_i \in [0,1]$.

The LP relaxation can be solved by LP solvers. In many cases, the solution to the relaxation teaches us something about the underlying ILP. One observation always holds true: the objective value of the relaxation is at least as large as the objective value of the underlying ILP; this assumes a maximization problem. The claim is trivial because any feasible solution to the ILP is also a feasible solution of the relaxation. The optimal solution to the LP relaxation will in general be *fractional*, i.e., variables take on rational values that are not integral. However, it might be the case that only a few variables have non-integral values. By appropriate rounding of fractional variables to integer values, we can often obtain good integer feasible solutions.

We give an example. The linear relaxation of the knapsack problem is given by:

$$\text{maximize } p \cdot x$$

subject to

$$w \cdot x \leq M, \quad \text{and} \quad x_i \in [0,1] \text{ for } i \in 1..n \enspace .$$

It has a natural interpretation. It is no longer required to add items completely to the knapsack, one can now take any fraction of an item. In our smuggling “scenario”, the *fractional knapsack problem* corresponds to the situation of divisible goods such as liquids or powders.

The fractional knapsack problem is easy to solve in time $\mathcal{O}(n \log n)$; there is no need for using a general purpose LP solver: Renumber (sort) the items by *profit density* such that

$$\frac{p_1}{w_1} \geq \frac{p_2}{w_2} \geq \cdots \geq \frac{p_n}{w_n} \ .$$

Find the smallest index j such that $\sum_{i=1}^{j} w_i > M$ (if there is no such index, we can take all knapsack items). Now set

$$x_1 = \cdots = x_{j-1} = 1, x_j = (M - \sum_{i=1}^{j-1} w_i)/w_j, \text{ and } x_{j+1} = \cdots = x_n = 0 \ .$$

Figure 12.1 gives an example. The fractional solution above is the starting point for many good algorithms for the knapsack problem. We will see more of this later.

Exercise 211 (Linear relaxation of the knapsack problem).

1. Prove that the above routine computes an optimal solution. Hint: you might want to use an *exchange argument* similar to the one used to prove the cut property of minimum spanning trees in Section 11.1.
2. Outline an algorithm that computes an optimal solution in linear expected time. Hint: use $\mathit{quickSelect}$ of Section 5.5.

A solution to the fractional knapsack problem is easily converted to a feasible solution of the knapsack problem. We simply take the fractional solution and round the sole fractional variable x_j to zero. We call this algorithm $\mathit{roundDown}$.

Exercise 212. Formulate the following *set covering* problem as an ILP: given a set M, subsets $M_i \subseteq M$ for $i \in 1..n$ with $\cup M_i = M$, and a cost c_i for each M_i. Select $F \subseteq 1..n$ such that $\bigcup_{i \in F} M_i = M$ and $\sum_{i \in F} c_i$ is minimized.

12.2 Greedy Algorithms — Never Look Back

The term *greedy algorithm* is used for a problem-solving strategy where the items under consideration are inspected in some order, usually some carefully chosen order, and the decision about the item, for example, whether to include it in the solution or not, is made when the item is considered. Decisions are never reversed. The algorithm for the fractional knapsack problem given in the preceding section follows the greedy strategy; we considered the items in decreasing order of profit density. The algorithms for shortest paths in Chapter 10 and for minimum spanning trees in Chapter 11 also follow the greedy strategy. For the single-source shortest path problem with non-negative weights we considered the edges in order of tentative distance of their source nodes. For these problems, the greedy approach led to an optimal solution.

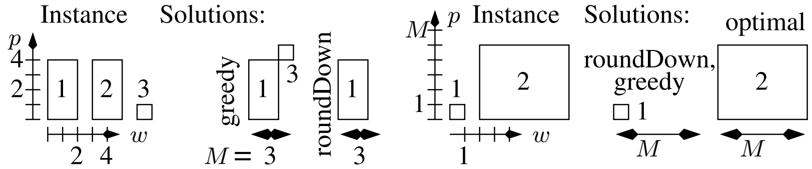


Fig. 12.3. Two instances of the knapsack problem. Left: For $p = (4, 4, 1)$, $w = (2, 2, 1)$, and $M = 3$ *greedy* performs better than *roundDown*. Right: For $p = (1, M - 1)$, $w = (1, M)$ both *greedy* and *roundDown* are far from optimal.

Usually, greedy algorithms only yield suboptimal solutions. Let us again consider the knapsack problem. A typical greedy approach would be to scan the items in order of decreasing profit density and to include items that still fit into the knapsack. We call this algorithm *greedy*. Figures 12.1 and 12.3 give examples. Observe that *greedy* always gives solutions at least as good as *roundDown*. Once *roundDown* encounters an item that it cannot include, it stops. However, *greedy* keeps on looking and often succeeds in including additional items of less weight. Although the example in Figure 12.1 gives the same result for both *greedy* and *roundDown*, they *are* different. For example, with profits $p = (4, 4, 1)$, weights $w = (2, 2, 1)$, and $M = 3$, *greedy* includes the first and third item yielding profit 5 whereas *roundDown* includes just the first item and only obtains profit 4. Both algorithms may produce solutions that are far from optimum. For example, for any capacity M consider the two item instance with profits $p = (1, M-1)$, and weights $w = (1, M)$. Both *greedy* and *roundDown* include only the first item which has high profit density but very small absolute profit. In this case it would be much better to include just item two.

We turn this observation into an algorithm which we call *round*. It computes two solutions: the solution x_d proposed by *roundDown* and the solution x_c choosing exactly the critical item x_j of the fractional solution. It then returns the better of the two.

We can give an interesting performance guarantee. Algorithm *round* always achieves at least 50 % of the profit of the optimal solution. More generally, we say that an algorithm achieves *approximation ratio* α if for all inputs, its solution is at most a factor α worse than the optimal solution.

Theorem 40. *Algorithm round achieves approximation ratio 2.*

Proof. Let x^* denote any optimal solution and let x_f be the optimal solution to the fractional knapsack problem. Then $p \cdot x^* \leq p \cdot x_f$. The objective function value is further increased by setting $x_j = 1$ in the fractional solution. We obtain

$$p \cdot x^* \leq p \cdot x_f \leq p \cdot x_d + p \cdot x_c \leq 2 \max \{p \cdot x_d, p \cdot x_c\} \quad .$$

There are many ways to refine algorithm *round* without sacrificing this approximation guarantee. We can replace x_d by the greedy solution. We can similarly augment x_c with any greedy solution for the smaller instance where item j is removed and the capacity is reduced by w_j.

We come to another important class of optimization problems, so-called *scheduling problems*. Consider the following scenario, known as the *scheduling problem for independent weighted jobs on identical machines*. We are given m identical machines on which we want to process n jobs; execution of job j takes t_j time units. An assignment $x : 1..n \to 1..m$ of jobs to machines is called a *schedule*. The maximum load assigned to any machine is called the *makespan* of the schedule, formally

$$L_{\max} = \max_{1\le j\le m} \sum_{i;\, x(i)=j} t_i \ .$$

The goal is to minimize the makespan of the schedule.

An application scenario is as follows. We have a video game processor with several identical processor cores. The jobs would be tasks of a video game such as audio processing, preparing graphics objects for the image processing unit, simulating physical effects, simulating the game intelligence, and so on.

We next give a simple greedy algorithm for the problem above that has the additional property that it does not need to know the job sizes in advance. We assign jobs in the order they arrive. Algorithms with this property are known as *online* algorithms. When job i arrives, we assign it to a machine with the smallest load. Formally, we compute the *loads* $\ell_j = \sum_{h<i\wedge x(h)=j} t_h$ of all machines j, and assign the new job to the most lightly loaded machine, i.e., $x(i) := j_i$ where j_i is such that $\ell_{j_i} = \min_{1\le j\le m} \ell_j$. This algorithm is frequently refered to as the *shortest queue algorithm*. It does not guarantee optimal solutions, but always computes nearly optimal solutions.

Theorem 41. *Shortest queue ensures* $L_{\max} \le \dfrac{1}{m}\displaystyle\sum_{i=1}^{n} t_i + \dfrac{m-1}{m}\max_{1\le i\le n} t_i$.

Proof. In the schedule generated by the shortest queue algorithm some machine has load $L_{\max}$. We focus on the job $\hat{\imath}$ that is the last job being assigned to the machine with maximum load. When job $\hat{\imath}$ is scheduled, all m machines have load at least $L_{\max} - t_{\hat{\imath}}$, i.e.,

$$\sum_{i\ne\hat{\imath}} t_i \ge (L_{\max} - t_{\hat{\imath}}) \cdot m \ .$$

Solving this for $L_{\max}$ yields

$$L_{\max} \le \frac{1}{m}\sum_{i\ne\hat{\imath}} t_i + t_{\hat{\imath}} = \frac{1}{m}\sum_{i} t_i + \frac{m-1}{m} t_{\hat{\imath}} \le \frac{1}{m}\sum_{i=1}^{n} t_i + \frac{m-1}{m}\max_{1\le i\le n} t_i \ .$$

We are almost finished. We only need to observe that $\sum_i t_i/m$ and $\max_i t_i$ are lower bounds on the makespan of any schedule and hence also the optimal schedule. We obtain:

Corollary 2. *Algorithm shortest queue achieves approximation ratio* $2 - 1/m$.

Proof. Let $L_1 = \sum_i t_i/m$ and $L_2 = \max_i t_i$. The makespan of the optimal solution is at least $\max(L_1, L_2)$. The makespan of the shortest queue solution is bounded by

$$L_1 + \frac{m-1}{m}L_2 \leq \frac{mL_1 + (m-1)L_2}{m} \leq \frac{(2m-1)\max(L_1, L_2)}{m}$$
$$= (2 - \frac{1}{m}) \cdot \max(L_1, L_2) .$$

Algorithm shortest queue is no better than claimed above. Consider an instance with $n = m(m-1)+1$, $t_n = m$, and $t_i = 1$ for $i < n$. The optimal solution has makespan $L_{\max}^{opt} = m$ whereas the shortest queue algorithm produces a solution with makespan $L_{\max} = 2m-1$. The shortest queue algorithm is an on-line algorithm. It produces a solution which is at most a factor $2 - 1/m$ worse than the solution produced by an algorithm that knows the entire input. In such a situation, we say that the online algorithm has *competitive ratio* $\alpha = 2 - 1/m$.

***Exercise 213** Show that the shortest queue algorithm achieves approximation ratio $4/3$ if the jobs are sorted by decreasing size.

***Exercise 214 (Bin packing.)** Suppose a smuggler boss has perishable goods in her cellar. She has to hire enough porters to ship all items tonight. Develop a greedy algorithm that tries to minimize the number of people she needs to hire assuming that they can all carry weight M. Try to show an approximation ratio for your *bin packing* algorithm.

Boolean formulae are another powerful description language. Here variables range over the boolean values `1` and `0` and the connectors $\wedge$, $\vee$, and $\neg$ are used to build formulae. A boolean formula is *satisfiable* if there is an assignment of boolean values to the variables such that the formula evaluates to `1`. We show how to formulate the pigeon-hole principle as a satisfiability problem: it is impossible to pack $n+1$ items into n bits such that every bin contains one item at most. We have variables x_{ij} for $1 \leq i \leq n+1$ and $1 \leq j \leq n$. So i ranges over items and j ranges over bins. Every item must be put into (at least) one bin, i.e., $x_{i1} \vee \ldots \vee x_{in}$ for $1 \leq i \leq n+1$. No bin should receive more than one item, i.e., $\neg(\vee_{1 \leq i < h \leq n+1} x_{ij}x_{hj})$ for $1 \leq j \leq n$. The conjunction of these formula is unsatisfiable. SAT solvers decide the satisfiability of boolean formulae.

Exercise 215. Formulate the pigeon-hole principle as an integer linear program.

12.3 Dynamic Programming — Building it Piece by Piece

For many optimization problems, the following *principle of optimality* holds: *An optimal solution is composed of optimal solutions to subproblems. If a subproblem has several optimal solutions, it does not matter which one is used.*

The idea behind dynamic programming is to build an exhaustive table of optimal solutions. We start with trivial subproblems. We build optimal solutions for increasingly larger problems by constructing them from the tabulated solutions to smaller problems.

Again, we use the knapsack problem as an example. Define $P(i, C)$ as the maximum profit possible when only items 1 to i can be put in the knapsack and the total weight is at most C. Our goal is to compute $P(n, M)$. We start with trivial cases and work our way up. The trivial cases are "no items" and "total weight zero". In both cases, the maximum profit it zero. So

$$P(0, C) = 0 \text{ for all } C \quad \text{and} \quad P(i, 0) = 0 \ .$$

Consider next the case $i > 0$ and $C > 0$. In the solution maximizing the profit we either use item i or we do not use it. In the latter case, the maximum achievable profit is $P(i-1, C)$. In the former case, the maximum achievable profit is $P(i-1, C-w_i) + p_i$ since we obtain profit p_i for item i and must use a solution of total weight at most $C - w_i$ for the first $i-1$ items. Of course, the former alternative is only feasible if $C \geq w_i$. We summarize the discussion in the following recurrence for $P(i, C)$:

$$P(i, C) = \begin{cases} \max(P(i-1, C), P(i-1, C-w_i) + p_i) & \text{if } w_i \leq C \\ P(i-1, C) & \text{if } w_i > C \end{cases} \tag{12.1}$$

Exercise 216. Show that the case distinction in the definition of $P(i, C)$ can be avoided by defining $P(i, C) = -\infty$ for $C < 0$.

Using the recurrence, we can compute $P(n, M)$ by filling a table $P(i, C)$ with one column for each possible capacity C and one row for each item i. Table 12.1 gives an example. There are many ways to fill this table, for example row by row. In order to reconstruct a solution from this table, we work our way backwards starting at the bottom right-hand corner of the table. Set $i = n$ and $C = M$. If $P(i, C) = P(i-1, C)$ we set $x_i = 0$ and continue in row $i-1$ with column C. Otherwise, we set $x_i = 1$. We have $P(i, C) = P(i-1, C-w_i) + p_i$ and therefore continue in row $i-1$ with column $C - w_i$. We continue with this procedure until we arrive at row 0 by which time the solution $(x_1, \ldots, x_n)$ has been completed.

Exercise 217. Dynamic programming, as described above, needs to store a table with $\Theta(nM)$ integers. Give a more space-efficient solution that stores only a single *bit* in each table entry except for two rows of $P(i, C)$ values at a time. What information is stored in this bit? How is it used to reconstruct a solution? How can you get down to *one* row of stored values? Hint: exploit your freedom in the order of filling in table values.

We will next describe an important optimization. It uses less space and is also faster. Instead of computing $P(i, C)$ for all i and all C, it only computes *Pareto-optimal* solutions. A solution x is Pareto-optimal if there is no solution that *dominates* it, i.e., has greater profit and no greater cost or the same profit and less cost. In

$i \setminus C$	0	1	2	3	4	5
0	0	0	0	0	0	0
1	**0**	10	10	10	10	10
2	0	10	10	**20**	30	30
3	0	10	15	25	30	**35**
4	0	10	15	25	30	**35**

Table 12.1. A dynamic programming table for the knapsack instance with $p = (10, 20, 15, 20)$, $w = (1, 3, 2, 4)$, and $M = 5$. Bold face entries contribute to the optimal solution.

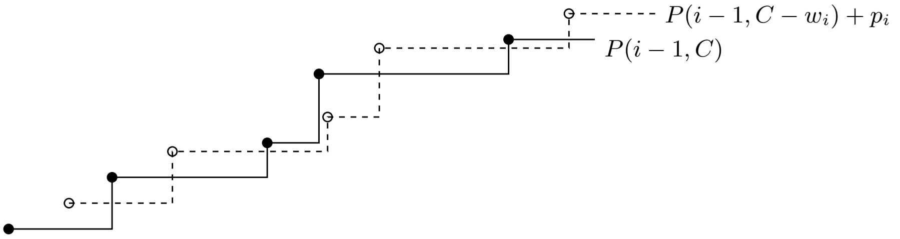


Fig. 12.4. The solid step function shows $C \mapsto P(i-1, C)$ and the dashed step function shows $C \mapsto P(i-1, C-w_i)+p_i$. $P(i, C)$ is the point-wise maximum of both functions. The solid step function is stored as the sequence of solid points. The representation of the dashed step function is obtained by adding (w_i, p_i) to every solid point. The representation of $C \mapsto P(i, C)$ is obtained by merging both representations and deleting all dominated elements.

other words, since $P(i, C)$ is an increasing function of C, we only need to remember those pairs $(C, P(i, C))$ where $P(i, C) > P(i, C-1)$. We store these pairs in a list L_i sorted by C value. So $L_0 = \langle(0, 0)\rangle$ indicating $P(0, C) = 0$ for all $C \geq 0$ and $L_1 = \langle(0, 0), (w_1, p_1)\rangle$ indicating that $P(1, C) = 0$ for $0 \leq C < w_1$ and $P(i, C) = p_1$ for $C \geq w_1$.

How can we go from L_{i-1} to L_i? The recurrence for $P(i, C)$ paves the way, see Figure 12.4. We have the list representation L_{i-1} for the function $C \mapsto P(i-1, C)$. We obtain the representation L'_{i-1} for $C \mapsto P(i-1, C-w_i)+p_i$ by shifting every point in L_{i-1} by (w_i, p_i). We merge L_{i-1} and L'_{i-1} into a single list by order of first component and delete all elements that are dominated by another value, i.e., we delete all elements that are preceded by an element with higher second component and for each fixed value of C, we keep only the element with largest second component.

Exercise 218. Give pseudo-code for the merge. Show that the merge can be carried out in time $|L_{i-1}|$. Conclude that the running time of the algorithm is proportional to the number of Pareto-optimal solutions.

The basic dynamic programming algorithm for the knapsack problem and also its optimization requires $\Theta(nM)$ worst case time. This is quite good if M is not too large. Since the running time is polynomial in n and M, the algorithm is called *pseudo-polynomial*. The "pseudo" means that it is not necessarily polynomial in the *input size* measured in bits; however, it is polynomial in the natural parameters n and M. There is, however, an important difference between the basic and the refined approach. The basic approach has best case running time $\Theta(nM)$. The best case for the refined approach is $O(n)$. The *average case* complexity of the refined algorithm is polynomial in n, independent of M. This even holds if the averaging is only done over perturbations of an arbitrary instance by small random noise. We refer the reader to [15] for details.

Exercise 219 (Dynamic Programming by Profit). Define $W(i, P)$ to be the smallest weight needed to achieve a profit of at least P using knapsack items $1..i$.

1. Show that $W(i, P) = \min\{W(i-1, P), W(i-1, P-p_i) + w_i\}$.
2. Develop a table-based dynamic programming algorithm using the above recurrence, that computes optimal solutions of the knapsack problem in time $\mathcal{O}(np^*)$ where p^* is the profit of the optimal solution. Hint: assume first that p^* is known or at least a good upper bound for it. Then remove this assumption.

Exercise 220 (Making Change). Suppose you have to program a vending machine that should give exact change using a minimum number of coins.

1. Develop an optimal greedy algorithm that works in the Euro zone with coins worth 1, 2, 5, 10, 20, 50, 100, and 200 cents and in the Dollar zone with coins worth 1, 5, 10, 25, 50, and 100 cents.
2. Show that this algorithm would not be optimal if there were a 4 cent coin.
3. Develop a dynamic programming algorithm that gives optimal change for any currency system.

Exercise 221 (Chained Matrix Products). We want to compute the matrix product $M_1 M_2 \cdots M_n$ where M_i is a $k_{i-1} \times k_i$ matrix. Assume that a pairwise matrix product is computed in the straight-forward way using mks element multiplications for the product of an $m \times k$ matrix with a $k \times s$ matrix. Exploit the associativity of matrix product to minimize the number of element multiplications needed. Use dynamic programming to find an optimal evaluation order in time $\mathcal{O}(n^3)$. For example, the product between a 4 × 5 matrix M_1, a 5 × 2 matrix M_2, and a 2 × 8 matrix M_3 can be computed in two ways. Computing $M_1(M_2 M_3)$ takes $5 \cdot 2 \cdot 8 + 4 \cdot 5 \cdot 8 = 240$ multiplications whereas computing $(M_1 M_2)M_3$ takes only $4 \cdot 5 \cdot 2 + 4 \cdot 2 \cdot 8 = 104$ multiplications.

Exercise 222 (Minimum Edit Distance). The *minimum edit distance* (or *Levenshtein distance*) $L(s, t)$ between two strings s and t is the minimum number of character deletions, insertions, and replacements applied to s that produces string t. For example, $L(\texttt{graph}, \texttt{group}) = 3$. (delete h, replace a by o, insert h before p). Define $d(i, j) = L(\langle s_1, \ldots, s_i \rangle, \langle t_1, \ldots, t_j \rangle)$. Show that

$$d(i, j) = \min\{d(i-1, j) + 1, d(i, j-1) + 1, d(i-1, j-1) + [s_i = t_j]\}$$

where $[s_i = t_j]$ is one if s_i is equal to t_j and is zero otherwise.

```
Function bbKnapsack($(p_1,\ldots,p_n),(w_1,\ldots,w_n),M) : \mathcal{L}$
    assert $p_1/w_1 \geq p_2/w_2 \geq \cdots \geq p_n/w_n$          // assume input sorted by profit density
    $\hat{x}$ = heuristicKnapsack($(p_1,\ldots,p_n),(w_1,\ldots,w_n),M)$ : $\mathcal{L}$     // best solution so far
    $x : \mathcal{L}$                                                   // current partial solution
    recurse$(1, M, 0)$
    return $\hat{x}$

    //Find solutions assuming $x_1,\ldots,x_{i-1}$ are fixed, $M' = M - \sum_{k<i} x_i w_i$, $P = \sum_{k<i} x_i p_i$.
    Procedure recurse$(i, M', P : \mathbb{N})$
        $u := P + upperBound((p_i,\ldots,p_n),(w_i,\ldots,w_n),M')$
        if $u > p \cdot \hat{x}$ then
            if $i > n$ then $\hat{x} := x$
            else                                                        // Branch on variable $x_i$
                if $w_i \leq M'$ then $x_i := 1$; recurse$(i+1, M' - w_i, P + p_i)$
                if $u > p \cdot \hat{x}$ then $x_i := 0$; recurse$(i+1, M', P)$
```

Fig. 12.5. A branch-and-bound algorithm for the knapsack problem. A first feasible solution is constructed by Function *heuristicKnapsack* using some heuristic algorithm. Function *upperBound* computes an upper bound for the possible profit.

Exercise 223. Does the principle of optimality hold for minimum spanning trees? Check the following three possibilities for definitions of subproblems: subsets of nodes, arbitrary subsets of edges, and prefixes of the sorted sequence of edges.

Exercise 224 (Constrained Shortest Path). Consider a directed graph $G = (V, E)$ where edges $e \in E$ have a *length* $\ell(e)$ and a *cost* $c(e)$. We want to find a path from node s to node t that minimizes the total length subject to the constraint that the total cost of the path is at most C. Show that subpaths $\langle s', t' \rangle$ of optimal solutions are *not* necessarily shortest paths from s' to t'.

12.4 Systematic Search — If in Doubt, Use Brute Force

In many optimization problems, the universe $\mathcal{U}$ of possible solutions is finite so that we can in principle solve the optimization problem by trying all possibilities. Naive application of this idea does not lead very far. However, we can frequently restrict the search to *promising* candidates and then the concept carries a lot further.

We will explain the concept of systematic search using the knapsack problem and a specific approach to systematic search known as *branch-and-bound*. In Exercises 226 and 227 we outline systematic search routines following a somewhat different pattern.

Figure 12.5 gives pseudo-code for a systematic search routine *bbKnapsack* for the knapsack problem. *Branching* is the most fundamental ingredient of systematic search routines. All sensible values for some piece of the solution are tried. For each of these values, the resulting problem is solved recursively. Within the recursive call,

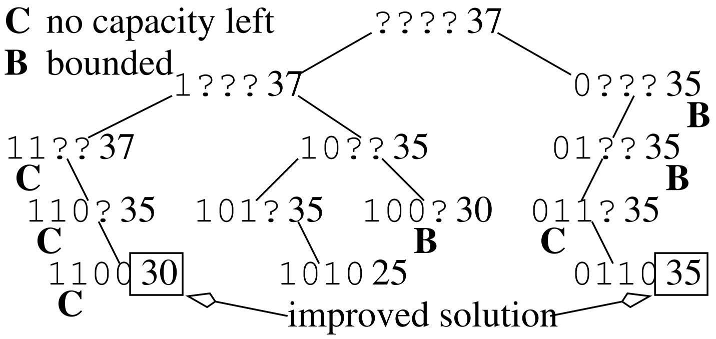


Fig. 12.6. The search space explored by *knapsackBB* for a knapsack instance with $p = (10, 20, 15, 20)$, $w = (1, 3, 2, 4)$, and $M = 5$, and empty initial solution $\hat{x} = (0, 0, 0, 0)$. The function *upperBound* is computed by rounding down the optimal objective function value of the fractional knapsack problem. The nodes of the search tree contain $x_1 \cdots x_{i-1}$ and the upper bound u. Left children are explored first and correspond to setting $x_i := 1$. There are two reasons for not exploring a child. Either if there is not enough capacity left to include an element (indicated by C) or if a feasible solution with profit equal to the upper bound is already known (indicated by B).

the chosen value is fixed. Routine *bbKnapsack* first tries including an item by setting $x_i := 1$ and then excluding it by setting $x_i := 0$. The variables are fixed one after the other in order of decreasing profit density. Assignment $x_i := 1$ is not tried if this would exceed the remaining knapsack capacity M'. With these definitions, after all variables are set, in the n-th level of recursion, *bbKnapsack* has found a feasible solution. Indeed, without the bounding rule below, the algorithm systematically explores *all* possible solutions and the *first* feasible solution encountered would be the solution found by algorithm *greedy*. The (partial) solutions explored by the algorithm form a tree. Branching happens at internal nodes of this tree.

Bounding is a method for pruning subtrees that cannot contain optimal solutions. A branch-and-bound algorithm keeps the best feasible solution found in a global variable $\hat{x}$; this solution is often called the *incumbent* solution. It is initialized to a solution determined by a heuristic routine and, at all times, provides a lower bound $p \cdot \hat{x}$ on the objective function value that can be obtained. This lower bound is complemented by an upper bound u for the objective function value obtainable by extending the current partial solution x to a full feasible solution. In our example, the upper bound could be the profit for the fractional knapsack problem with items $i..n$ and capacity $M' = M - \sum_{j<i} x_i w_i$.

Branch-and-bound stops expanding the current branch of the search tree when $u \leq p \cdot \hat{x}$, i.e., when there is no hope for an improved solution in the current subtree of the search space. Why do we test $u > p \cdot \hat{x}$ twice in procedure *recurse*? The reason is that the case $x_i := 1$ might lead to an improved feasible solution whose profit matches the upper bound. Then there is no need to explore the case $x_i := 0$.

Exercise 225. Explain how to implement the function $upperBound$ in Figure 12.5 so that it runs in time $\mathcal{O}(\log n)$. Hint: precompute prefix sums $\sum_{k\leq i} w_i$ and $\sum_{k\leq i} p_i$ and use binary search.

Solving Integer Linear Programs: In Section 12.1.1 we have seen how to formulate the knapsack problem as a 0-1 integer linear program. We will now indicate how the branch-and-bound procedure developed for the knapsack problem can be applied to any 0-1 integer linear program. Recall that in a 0-1 integer linear program the values of the variables are constrained to 0 and 1. Our discussion will be brief and we refer the reader to a textbook on integer linear programming [139, 162] for more information.

The main change is that function $upperBound$ now solves a general linear program that has variables x_i,…,x_n with range $[0, 1]$. The constraints for this LP come from the input ILP with variables x_1 to x_{i-1} replaced by their values. In the remainder of this section we will simply refer to this linear program as "the LP".

If the LP has a feasible solution, $upperBound$ returns the optimal value of the LP. If the LP has no feasible solution, $upperBound$ returns $-\infty$ so that the ILP solver will stop exploring this branch of the search space. We will next describe several generalizations of the basic branch-and-bound procedure that sometimes lead to considerable improvements.

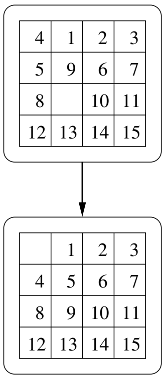
Branch Selection: We may pick any unfixed variable x_j for branching. In particular, we can make the choice depend on the solution of the LP. A commonly used rule is to branch on a variable whose fractional value in the LP is closest to $1/2$.

Order of Search Tree Traversal: In the knapsack example the search tree was traversed depth first and the 1-branch was tried first. In general, we are free to choose any order of tree traversal. There are at least two considerations influencing the choice of strategy. As long as no good feasible solution is known, it is good to use a depth-first strategy so that complete solutions are explored quickly. Otherwise, a *best-first* strategy is better that explores those search tree nodes that are most likely to contain good solutions. Search tree nodes are kept in a priority queue and the next node to be explored is the most promising node in the queue. The priority could be the upper bound returned by the LP. Since the LP is expensive to evaluate, one sometimes settles for an approximation.

Finding Solutions: We may be lucky and the solution of the LP turns out to assign integer values to all variables. In this case there is no need for further branching. Application specific heuristics can additionally help to find good solutions quickly.

Branch-and-Cut: When an ILP solver branches too often, the size of the search tree explodes and it becomes too expensive to find an optimal solution. One way to avoid branching is to add constraints to the linear program that *cut* away solutions with fractional values for the variables without changing the solutions with integer values.

Exercise 226 (15-puzzle). The 15-puzzle is a popular sliding-block puzzle. You have to move 15 square tiles in a 4×4 frame into the right order. Define a move as the action of interchanging a square and the hole.



4	1	2	3
5	9	6	7
8		10	11
12	13	14	15

	1	2	3
4	5	6	7
8	9	10	11
12	13	14	15

Design a systematic search algorithm that finds a shortest move sequence from a given starting configuration to the ordered configuration shown at the bottom. Use *iterative deepening depth first search* [111]: Try all one move sequences first, then all two move sequences, and so on. This should work for the simpler 8-puzzle. For the 15-puzzle use the following optimizations: never undo the immediately preceding move. Maintain the number of moves that would be needed if all pieces could be moved freely. Stop exploring a subtree if this bound proves that the current search depth is too small. Decide beforehand, whether the number of moves is odd or even. Implement your algorithm to run in constant time per move tried.

Exercise 227 (Constraint programming and the eight queens problem). Consider an 8×8 checkerboard. The task is to place 8 queens on the board so that they do not attack each other, i.e., no two queens should be placed in the same row, column, diagonal or anti-diagonal. So each row contains exactly one queen. Let x_i be the position of the queen in row i. Then $x_i \in 1..8$. The solution must satisfy the following constraints: $x_i \neq x_j$, $i + x_i \neq j + x_j$, and $x_i - i \neq x_j - j$ for $1 \leq i < j \leq 8$. What do these conditions express? Show that they are sufficient. A systematic search can use the following optimization. When a variable x_i is fixed to some value, this excludes values for variables that are still free. Modify systematic search so that it keeps track of the values that are still available for free variables. Stop exploration as soon as there is a free variable that has no value available to it anymore. This technique of eliminating values is basic to *constraint programming*.

12.5 Local Search — Think Globally, Act Locally

The optimization algorithms we have seen so far are only applicable in special circumstances. Dynamic programming needs a special structure of the problem and may require a lot of space and time. Systematic search is usually too slow for large inputs. Greedy algorithms are fast but often yield only low-quality solutions. *Local search* is a widely applicable iterative procedure. It starts with some feasible solution and then moves from feasible solution to feasible solution by local modifications. Figure 12.7 gives the basic framework. We will refine it later.

Local search maintains a current feasible solution x and the best solution $\hat{x}$ seen so far. In each step, local search moves from the current solution to a neighboring solution. What are neighboring solutions? Any solution that can be obtained from the current solution by making small changes to it. For example, in the knapsack problem, we might remove up to two items from the knapsack and replace them by

```
find some feasible solution $x \in \mathcal{L}$
$\hat{x} := x$                                          // $\hat{x}$ is best solution found so far
while not satisfied with $\hat{x}$ do
    $x :=$ some heuristically chosen element from $\mathcal{N}(x) \cap \mathcal{L}$
    if $f(x) < f(\hat{x})$ then $\hat{x} := x$
```

Fig. 12.7. Local search.

up to two other items. The precise definition of the neighborhood depends on the application and the algorithm designer. In the framework, we use $\mathcal{N}(x)$ to denote the *neighborhood* of x. The second important design decision is which solution from the neighborhood is chosen. Finally, some heuristic decides when to stop.

In the next sections, we will tell you more about local search.

12.5.1 Hill Climbing

Hill climbing is the greedy version of local search. It only moves to neighbors that are better than the currently best solution. This restriction further simplifies local search. The variables $\hat{x}$ and x are the same and we stop when no improved solutions are in the neighborhood $\mathcal{N}$. The only non-trivial aspect of hill climbing is the choice of the neighborhood. We will give two examples where hill climbing works quite well followed by an example where it fails badly.

Our first example is the traveling salesman problem from Section **??**[ps: changed $\Longrightarrow$ reference (was spath)]. Given an undirected graph and a distance function on the edges satisfying the triangle inequality, the goal is to find a shortest tour visiting all nodes of the graph. We define the neighbors of a tour as follows. Let (u, v) and (w, y) be two edges of the tour, i.e., the tour has the form $(u, v), p, (w, y), q$, where p is a path from v to w and q is a path from y to u. We remove the two edges from the tour and replace them by the edges (u, w) and (v, y). The new tour first traverses (u, w), then uses the reversal of p back to v, then uses (v, y) and finally traverses q back to u. This move is known as a 2-exchange and a tour that cannot be improved by a 2-exchange is called 2-optimal. In many instances of the traveling salesman problem, 2-optimal tours come quite close to optimum tours.

Exercise 228. Describe a scheme where three edges are removed and replaced by new edges.

An interesting example of hill climbing with a clever choice of the neighborhood function is the *simplex algorithm* for linear programming (see Section 12.1). It is the most widely used algorithm for linear programming. The set of feasible solutions $\mathcal{L}$ of a linear program is defined by a set of linear equalities and inequalities $a_i \cdot x \bowtie b_i$, $1 \leq i \leq m$. The points satisfying a linear equality $a_i \cdot x = b_i$ form a hyperplane in R^n and the points satisfying a linear inequality $a_i \cdot x \leq b_i$ or $a_i \cdot x \geq b_i$ form a halfspace. Hyperplanes are the n-dimensional analogues of planes and half-spaces are the analogues of half-planes. The set of feasible solutions is the

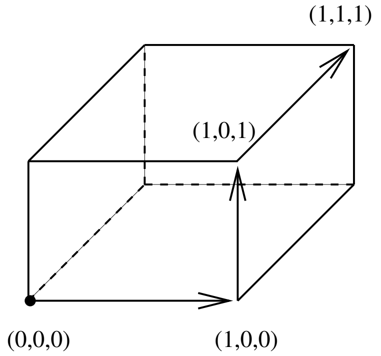


Fig. 12.8. The 3-dimensional unit-cube is defined by the inequalities $x \geq 0$, $x \leq 1$, $y \geq 0$, $y \leq 1$, $z \geq 0$, and $z \leq 1$. In the vertices $(1, 1, 1)$ and $(1, 0, 1)$ three inequalities are tight and on the edge connecting these vertices the inequalities $x \leq 1$ and $z \leq 1$ are tight. For the objective "maximize $x + y + z$", the simplex algorithm starting in $(0, 0, 0)$ may move along the path indicated by arrows. The vertex $(1, 1, 1)$ is optimal since the half-space $x+y+z \leq 3$ contains the entire feasible region and has $(1, 1, 1)$ in its boundary.

intersection of m half-spaces and hyperplanes and forms a *convex polytope*. We have already seen an example in two dimensional space in Figure 12.2. Figure 12.8 shows an example in three dimensional space. Convex polytopes are the n-dimensional analogues of convex polygons. In the interior of the polytope all inequalities are strict (= satisfied with inequality), on the boundary some inequalities are tight (= satisfied with equality). The vertices and edges of the polytope are particularly important parts of the boundary. In the vertices, n inequality constraints are tight, and on the edges, $n - 1$ inequalities are tight [4]. Please verify this statement for Figures 12.2 and 12.8.

The simplex algorithm starts in an arbitrary vertex of the feasible region. In each step it moves to a neighboring vertex, i.e., a vertex reachable via an edge, with larger objective value. If there is more than one such neighbor, a common strategy moves to the neighbor with largest objective value. If there is no neighbor with a larger objective value, the algorithm stops. *At this point, it has found the vertex with maximal objective value.* In the examples in Figures 12.2 and 12.8, the captions argue why this is true. The general argument is as follows. Let x^* be the vertex at which the simplex algorithm stops. The feasible region is contained in the cone with apex x^* and spanned by the edges incident to x^*. All these edges go to vertices with smaller objective values and hence the entire cone is contained in the half-space $c \cdot x \leq c \cdot x^*$. Thus no feasible point can have an objective value larger than x^*. We described the simplex algorithm as a walk on the boundary of a convex polytope, i.e, in geomet-

[4] This statement assumes that the constraints are in general position and that there are no equality constraints. Equality constraints can be used to eliminate a variable and so there is no harm in restricting the argument to inequality constraints.

```
find some feasible solution $x \in \mathcal{L}$
$T$:= some positive value                                   // initial temperature of the system
while $T$ is still sufficiently large do
    perform a number of steps of the following form
        pick $x'$ from $\mathcal{N}(x) \cap \mathcal{L}$ uniformly at random
        with probability $\min(1, \exp(\frac{f(x')-f(x)}{T})$ do $x := x'$
    decrease $T$                                  // make moves to inferior solutions less likely
```

Fig. 12.9. Simulated Annealing

ric language. It can be equivalently described using the language of linear algebra. Actual implementations use the linear algebra description.

In the case of linear programming, hill climbing leads to an optimal solution. In general, hill climbing will not find an optimal solution. In fact, it will not even find a near optimal solution. Consider the following example. Our task is to find the highest point on earth, i.e., Mount Everest. A feasible solution is any point on earth. The local neighborhood of a point is any point within a distance of 10 kilometers. So the algorithm would start at some point on earth, then go to the highest point within a distance of 10 kilometers, then again go to the highest point within a distance of 10 kilometers, and so on. If one starts from the first of author's home (altitude 206 meters), the first step would lead to an altitude 350 meters, and there the algorithm would stop, because there is no higher hill within 10 kilometers from it. There are very few places in the world, where the algorithm would continue for long, and even fewer places, where it would find Mount Everest.

Why does hill climbing work so nicely for linear programming, but fails to find Mount Everest. The reason is that the earth has many local optima, hills that are highest within a range of 10 kilometers. On the contrary, a linear program has only one local optimum (which then, of course, is also a global optimum). For a problem with many local optima, we should expect any generic method to have difficulties. Observe that increasing the size of the neighborhoods in the search for Mount Everest does not really solve the problem, except if neighborhoods are made to cover the entire earth. But then finding the optimum in a neighborhood is as hard as the full problem.

12.5.2 Simulated Annealing — Learning from Nature

If we want to ban the bane of local optima in local search, we must find a way to escape from them. This means that we sometimes have to accept moves that decrease the objective value. What could 'sometimes' mean in this context? We have contradicting goals. On the one hand, we must be willing to make many downhill steps so that we can escape from wide local optima. On the other hand, we must be sufficiently target-oriented so that we find a global optimum at the end of a long narrow ridge. A very popular and successful approach for reconciling the contradicting goals is *simulated annealing*, see Figure 12.9. It works in phases that are controlled

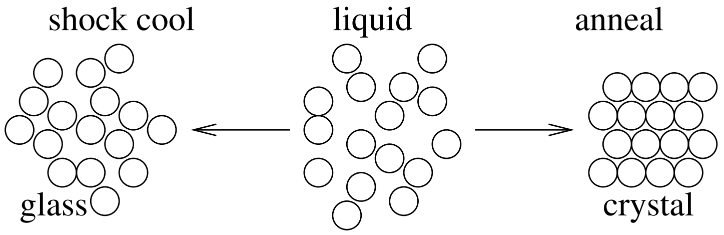


Fig. 12.10. Annealing versus Shock Cooling.

by a parameter T, called the *temperature* of the process. We will explain below why the language of physics is used in the description of simulated annealing. In each phase, a number of moves are made. In each move, a neighbor $x' \in \mathcal{N}(x) \cap \mathcal{L}$ is chosen uniformly at random and the move from x to x' is made with a certain probability. This probability is one, if x' improves upon x. This probability is less than one if the move is to an inferior solution. The trick is to make the probability depend on T. If T is large, we make the move relatively likely, if T is close to zero, we make the move relatively unlikely. The hope is that in this way, the process zeroes in on a region of a good local optimum in phases of high temperature and then actually finds a near-optimal solution in the phases of small temperature. The exact choice of transition probability in the case that x' is an inferior solution is given by $\exp((f(x') - f(x)/T)$. Observe that T is in the denominator and that $f(x') - f(x)$ is negative. So the probability decreases with T and also with the absolute loss in objective value.

Why is the language of physics used and why this apparently strange choice of transition probabilities? Simulated annealing is inspired by the physical process of *annealing* that can be used to minimize[5] the global energy of a physical system. For example, consider a pot of molten silica ($\mathrm{SiO_2}$), see Figure 12.10. If we cool it very quickly, we obtain glass — an amorphous substance in which every molecule is in a local minimum of energy. This process of shock cooling has a certain similarity to hill climbing. Every molecule simply drops into a state of locally minimal energy; in hill climbing, we accept a local modification of state, if it leads to a smaller value of the objective function. However, glass is not a state of global minimum energy. A much lower state of energy is reached by a quartz crystal in which all molecules are arranged in a regular way. This state can be reached (or approximated) by cooling the melt very slowly and even slightly reheating it from time to time. This process is called *annealing*. How can it be that molecules arrange into perfect shape over a distance of billions of molecule diameters although they feel only local forces extending over a few molecule diameters?

Qualitatively, the explanation is that local energy minima have enough time to dissolve in favor of globally more efficient structures. For example, assume that a cluster of a dozen molecules approaches a small perfect crystal that already consists

[5] Note that we are talking about minimization now.

of thousands of molecules. Then with enough time and the help of reheating, the cluster will dissolve and its molecules can attach to the crystal. Here is a more formal description of this process that can be shown to hold within a reasonable model of the system: if cooling is sufficiently slow, the system reaches *thermal equilibrium* at every temperature. Equilibrium at temperature T means that a state x of the system with energy E_x is assumed with probability

$$\frac{\exp(-E_x/T)}{\sum_{y\in\mathcal{L}}\exp(-E_y/T)}$$

where T is the temperature of the system and $\mathcal{L}$ is the set of system states. This energy distribution is called *Boltzmann* distribution. When T decreases, the probability of states with minimal energy grows. Actually, in the limit $T \to 0$, the probability of states with minimal energy approaches one.

The same mathematics works for abstract systems corresponding to a maximization problem. We identify the cost function f with the energy of the system and a feasible solution with the state of the system. It can be shown that the system approaches a Boltzmann distribution for a quite general class of neighborhoods and the following rules for choosing the next state:

```
pick $x'$ from $\mathcal{N}(x) \cap \mathcal{L}$ uniformly at random
with probability $\min(1, \exp(\frac{f(x')-f(x)}{T})$ **do** $x := x'$
```

The physical analogy gives some idea of why simulated annealing might work[6], but it does not provide an implementable algorithm. We have to get rid of two infinities: for every temperature, wait infinitely long to reach equilibrium, and do that for infinitely many temperatures. Simulated annealing algorithms therefore have to decide on a *cooling schedule*, i.e., how the temperature T should be varied over time. A simple schedule chooses a starting temperature T_0 that is supposed to be just large enough so that all neighbors are accepted. Furthermore, for a given problem instance there is a fixed number N of iterations used at each temperature. The idea is that N should be as small as possible but still allow the system to get close to equilibrium. After every N iterations, T is decreased by multiplying it with a constant α less than one. Typically, α is between 0.8 and 0.99. When T has become so small that moves to inferior solutions have become highly unlikely (this is the case then T is comparable to the smallest difference in objective value between any two feasible solutions), T is finally set to 0, i.e, the annealing process concludes with a hill climbing search.

Better performance can be obtained with *dynamic schedules*. For example, the initial temperature can be determined by starting with a low temperature and increasing it quickly until the fraction of accepted transitions approaches one. Dynamic schedules base their decision on how much T should be lowered on the actually observed variation in $f(x)$ during local search. If the temperature change is tiny compared to the variation, it has too little effect. If the change is too close to or even larger than the variation observed, there is the danger that the system is prematurely forced into a local optimum. The number of steps to be made until the temperature

[6] Note that we wrote “might work” and not “works”.

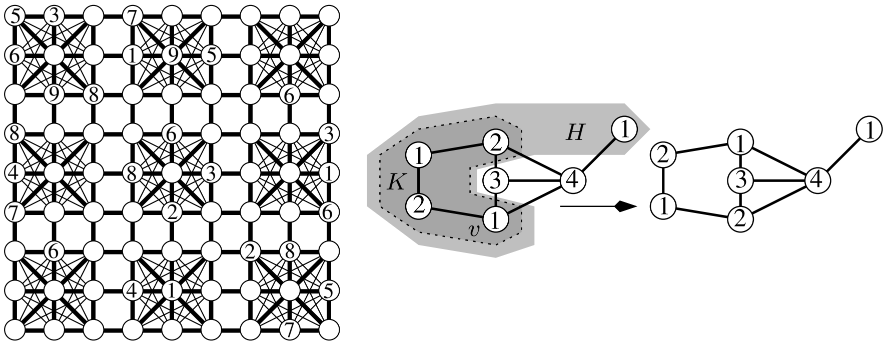


Fig. 12.11. The figure on the left shows a partial coloring of the graph underlying Sudoku puzzles. The bold straight line segments indicate cliques consisting of all nodes touched by the line. The figure on the right shows a step of Kempe Chain annealing using colors 1 and 2 and node v.

is lowered can be made dependent on the actual number of accepted moves. Furthermore, one can use a simplified statistical model of the process to estimate when the system approaches equilibrium. The details of dynamic schedules are beyond the scope of this exposition.

Exercise 229. Design a simulated annealing algorithm for the knapsack problem. The local neighborhood of a feasible solution are all solutions that can be obtained by removing up to two elements and then adding up to two elements.

We exemplify simulated annealing on the so-called *graph coloring problem*. For an undirected graph $G = (V, E)$, a *node coloring* with k colors is an assignment $c : V \to 1..k$ such that no two adjacent nodes get the same color, i.e., $c(u) \neq c(v)$ for all edges $\{u, v\} \in E$. There is always a solution with $k = |V|$ colors; we simply give each node its own color. The goal is to minimize k. There are many applications for graph coloring and related problems. The most "classical" one is map coloring — the nodes are countries and edges indicate that these countries have a common border and thus should not be rendered in the same color. A famous theorem of graph theory states that all maps (i.e. planar graphs) can be colored with at most four colors [152]. *Sudoku* puzzles are a well-known instance of the graph coloring problems, where the player is asked to complete a partial coloring of the graph shown in Figure 12.11 with the digits $1..9$. We will present two simulated annealing approaches to graph coloring; many more have been tried.

Kempe Chain Annealing: Of course, the obvious objective function for graph coloring is the number of colors used. However, this choice of objective function is too simplistic in a local search framework, since a typical local move will not change the number of colors used. We need an objective function that rewards local changes that are "on a good way" towards using fewer colors. One such function is the sum of the squared sizes of the color classes. Formally, let $C_i = \{v \in V : c(v) = i\}$ be the set of nodes that are colored i. Then

$$f(c) = \sum_i |C_i|^2 .$$

This objective function is to be maximized. Observe that the objective function increases when a large color class is further enlarged at the cost of a small color class. Thus local improvements will eventually empty some color classes, i.e., the number of colors decreases.

Having settled the objective function, we come to the definition of local change or neighborhood. A trivial definition is as follows: a local change consists in recoloring a single vertex; it can be given any color not used on one of its neighbors. Kempe chain annealing uses a more liberal definition of "local recoloring". Kempe was one of the early investigators of the four-color problem; he invented Kempe chains in his futile proof attempts. Assume our goal it to recolor node v with current color $i = c(v)$ to color j. In order to maintain feasibility, we have to change some other node colors too: node v might be connected to nodes currently colored j. So we color these nodes with color i. These nodes might in turn be connected to other nodes of color j and so on. More formally, consider the node induced subgraph H of G which contains all nodes with colors i and j. The connected component of H that contains v is the *Kempe Chain* K we are interested in. We maintain feasibility by swapping colors i and j in K. Figure 12.11 gives an example. Kempe chain annealing starts with any feasible coloring.

Exercise 230. Use Kempe chains to prove that any planar graph G can be colored with five colors. Hint: use the fact that a planar graph is guaranteed to have a node of degree five or less. Let v be any such node. Remove it from G and color $G - v$ recursively. Put v back it. If at most four different colors are used on the neighbors of v, there is a free color for v. So assume otherwise. Assume w.l.o.g. that the neighbors of v are colored with colors 1 to 5 in clockwise order. Consider the subgraph of nodes colored 1 and 3. If the neighbors of v with colors 1 and 3 are in distinct connected components of this subgraph, a Kempe chain can be used to recolor the node colored 1 with color 3. If they are in the same component, consider the subgraph of nodes colored 2 and 4. Argue that the neighbors of v with colors 2 and 4 must be in distinct components of this subgraph.

The Penalty Function Approach: A generally useful idea for local search is to relax some of the constraints on feasible solutions in order to make the search more flexible and in order to ease the discovery of a starting solution. Observe, that we assumed so far somehow having a feasible solution available to us. However, in some situations finding any feasible solution is already a hard problem; the eight queens problem from Exercise 227 is an example. In order to obtain a feasible solution in the end, the objective function is modified to penalize infeasible solutions. The constraints are effectively moved into the objective function.

In the graph coloring example, we now also allow illegal colorings, i.e., colorings in which neighboring nodes may have the same color. An initial solution is generated by guessing the number of colors needed and coloring the nodes randomly. A neighbor of the current coloring c is generated by picking a random color j and a random node v colored j, i.e, $x(v) = j$. Then, a random new color for node v is chosen among all the colors already in use plus one fresh, previously unused color.

As above, let C_i be the set of nodes colored i and let $E_i = E \cap C_i \times C_i$ be the set of edges connecting two nodes in C_i. The objective is to minimize

$$f(c) = 2\sum_i |C_i| \cdot |E_i| - \sum_i |C_i|^2 \ .$$

The first term penalizes illegal edges; each illegal edge connecting two nodes of color i contributes the size of the i-th color class. The second favors large color classes as we have already seen above. The objective function does not necessarily have its global minimum at an optimal coloring, however, local minima are legal colorings. Hence, the penalty version of simulated annealing is guaranteed to find a legal coloring even if it starts with an illegal coloring.

Exercise 231. Show that the objective function above has its local minima at legal colorings. Hint: consider the change of $f(c)$ if one end of a legally colored edge is recolored with a fresh color? Prove that the objective function above does not necessarily have its global optimum at a solution using the minimal number of colors.

Experimental Results: Johnson et al. [99] performed a detailed study of algorithms for graph coloring with particular emphasis on simulated annealing. We will briefly report on their findings and then draw some conclusions. Most of their experiments were performed on random graphs in the so-called $G_{n,p}$-model or on random geometric graphs.

In the $G_{n,p}$-model, where p is a parameter in $[0, 1]$, an undirected random graph on n nodes is built by adding each of the $n(n-1)/2$ candidate edges with probability p. The experiments for distinct edges are independent. In this way, the expected degree of every node is $p(n-1)$ and the expected number of edges is $pn(n-1)/2$. For random graphs with 1000 nodes and edge probability 0.5, Kempe chain annealing produces very good colorings given enough time. However, a sophisticated and expensive greedy algorithm, *XRLF*, produces even better solutions in less time. For very dense random graphs with $p = 0.9$, Kempe chain annealing performed better than XRLF. For sparser random graphs with edge probability 0.1, *penalty function annealing* outperforms Kempe chain annealing and can sometimes compete with XRLF.

Another interesting class of random inputs are *random geometric graphs*: choose n random uniformly distributed points in the unit square $[0, 1] \times [0, 1]$. They represent the nodes of the graph. Connect two points by an edge if their Euclidean distance is at most some given range r. Figure 12.12 gives an example. Such instances are frequently used to model applications where nodes are radio transmitters and colors are frequency bands. Nodes that lie within distance r from one another must not use the same frequency to avoid interference. For this model, Kempe chain annealing is performed well, but was outperformed by a third annealing strategy called *fixed-K annealing*.

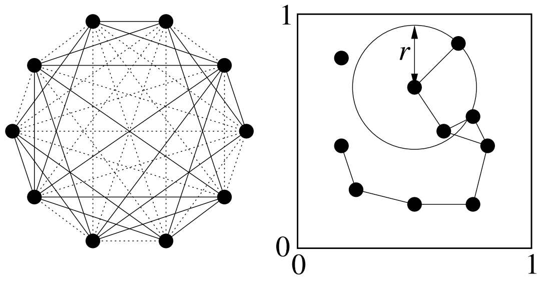


Fig. 12.12. Left: A random graph with 10 nodes and $p = 0.5$. Edges chosen are drawn solid, edges rejected are drawn dashed. Right: A random geometric graph with 10 nodes and range $r = 0.27$.

What should we learn from this? The relative performance of simulated annealing approaches strongly depends on the class of inputs and the available computing time. Moreover, it is impossible to make predictions about the performance on an instance class based on experience from other instance classes. So be warned. Simulated annealing is a heuristic and, as for any other heuristic, you should not make claims about its performance on an instance class before having tested it extensively on it.

12.5.3 More on Local Search

We close our treatment of local search with the discussion of two refinements that can be used to modify or replace the approaches presented so far.

⟹ [todo: threshold acceptance verstÃď’ndlicher machen]

Threshold Acceptance: There seems to be nothing magic about the particular form of the acceptance rule of simulated annealing. For example, a simpler yet also successful rule uses the parameter T as a threshold. New states with a value $f(x)$ below the threshold are accepted others are not.

Tabu Lists: Local search algorithms sometimes return to the same suboptimal solution again and again — they cycle. For example, simulated annealing might have reached the top of a steep hill. Randomization will steer the search away from the optimum but the state may remain on the hill for a long time. *Tabu search* steers away from local optima by keeping a *Tabu list* of “solution elements” that should be “avoided” in new solutions for the time being. For example, in graph coloring a search step could change the color of a node v from i to j and then store the tuple (v, i) in the Tabu list to indicate that color i is forbidden for v as long as (v, i) is in the Tabu list. Usually, this Tabu condition is not applied if an improved solution is obtained by coloring node v with color i. Tabu lists are so successful that they can be used as the core technique of an independent variant of local search called *Tabu search*.

Restarts: The typical behavior of a well-tuned local search algorithm is that it moves to an area with good feasible solutions and then explores this area trying to find better and better local optima. However, it might be that there are other, far away areas with much better solutions. The search for Mount Everest illustrates the point. If we start in Australia, the best we can hope for is to end up at Mount Kosciuszko (altitude 2229 m), a solution far from optimum. It therefore makes sense to run the algorithm multiple times with different random starting solutions because it is likely that different starting points will explore different areas of good solutions. Starting the search for Mount Everest at multiple locations and in all continents will certainly lead to a better solution than just starting in Australia. Even if these restarts do not improve the average performance of the algorithm, they may make it more robust in the sense that it is less likely to produce grossly suboptimal solutions. Several independent runs are also an easy source of parallelism. Just run the program on different workstations concurrently.

12.6 Evolutionary Algorithms

Living beings are ingeniously adaptive to their environment and master the problems encountered in daily life with great ease. Can we somehow use the principles of life for developing good algorithms? The theory of evolution tells us that the mechanisms leading to this performance are *mutation*, *recombination*, and *survival of the fittest*. What could an evolutionary approach mean for optimization problems?

The genome describing an individual corresponds to the description of a feasible solution. We can also interpret infeasible solutions as dead or ill individuals. In nature, it is important that there is a sufficiently large *population* of genomes; otherwise, recombination deteriorates to incest and survival of the fittest cannot demonstrate its benefits. So, instead of one solution as in local search, we are now working with a pool of feasible solutions.

The individuals in a population produce offsprings. Because resources are limited, individuals better adapted to the environment are more likely to survive and to produce more offsprings. In analogy, feasible solutions are evaluated using a fitness function f, and fitter solutions are more likely to survive and to produce offsprings. Evolutionary algorithms usually work with a solution pool of limited size, say N. Survival of the fittest can then be implemented as keeping only the best N solutions.

Even in bacteria which reproduce by cell division, no offspring is identical to its parent. The reason is *mutation*. When a genome is copied, small errors happen. Although mutations usually have an adverse effect on fitness, some also improve fitness. Local changes of a solution are the analogy of mutations.

In evolution, an even more important ingredient is *recombination*. Offsprings contain genetic information from both parents. The importance of recombination is easy to understand if one considers how rare useful mutations are. Therefore it takes much longer to obtain an individual with two new and useful mutations than it takes to combine two individuals with two different useful mutations.

```
Create an initial population $population = \{x_1, \ldots, x_N\}$
while not finished do
    if matingStep then
        select individuals $x_1$, $x_2$ with high fitness and produce $x' := mate(x_1, x_2)$
    else select an individual $x_1$ with high fitness and produce $x' = mutate(x_1)$
    $population := population \cup \{x'\}$
    $population := \{x \in population : x$ is sufficiently fit$\}$
```

Fig. 12.13. A generic evolutionary algorithm.

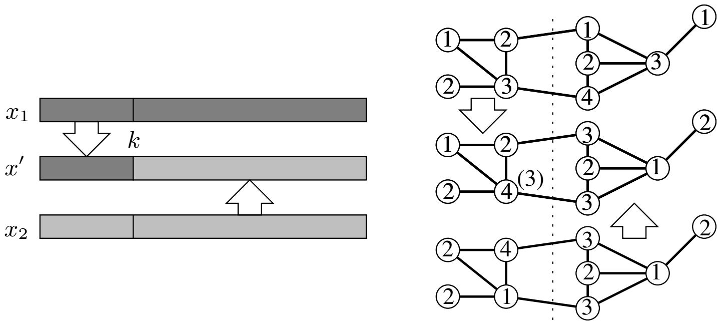


Fig. 12.14. Mating using crossover (left) and by stitching together pieces of a graph coloring (right).

We now have all the ingredients needed for a generic evolutionary algorithm, see Figure 12.13. As for the other approaches presented in this chapter, many details need to be filled in before obtaining an algorithm for a specific problem. The algorithm starts by creating an initial population of size N. This process should involve randomness but it is also useful to use heuristics that produce good initial solutions.

In the loop, it is first decided whether an offspring should be produced by mutation or by recombination. This is a probabilistic decision. Then one or two individuals are chosen for reproduction. To put selection pressure on the population, it is important to base reproduction success on the fitness of the individuals. However, usually it is not desirable to draw a hard line and only use the fittest individuals because this might lead to a too uniform population and incest. For example, one can choose reproduction candidates randomly giving a higher selection probability to fitter individuals. An important design decision is how to fix these probabilities. One choice is to sort the individuals by fitness and then to define the reproduction probability as some decreasing function of rank. This indirect approach has the advantage that it is independent of the objective function f and the absolute fitness differences between individuals which is likely to decrease during the course of evolution.

The most critical operation is mate which produces new offsprings from two ancestors. The "canonical" mating operation is called *crossover*: individuals are assumed to be represented by a string of n bits. Choose an integer k. The new individual takes the first k bits from one parent and the last $n - k$ bits from the other parent. Figure 12.14 shows this procedure. Alternatively, one may choose k random positions from the first parent and the remaining bits from the other parent. For our knapsack example, crossover is a quite natural choice. Each bit decides whether the corresponding item is in the knapsack or not. In other cases, crossover is less natural or would require a very careful encoding. For example, for graph coloring it seems more natural to cut the graph in two pieces such that few edges are cut. Now one piece inherits its colors from the first parent and the other piece inherits them from the other parent. Some of the edges running between the pieces might now connect nodes with the same color. This could be repaired using some heuristics, e.g., choosing the smallest legal color for mis-colored nodes in the part corresponding to the first parent. Figure 12.14 gives an example.

Mutations are realized as in local search. In fact, local search is nothing but an evolutionary algorithm with population size one.

The simplest way to limit the size of the population is to keep it fixed by removing the least fit individual in each iteration. Other approaches that give room to different "ecological niches" can also be used. For example, for the knapsack problem one could keep all Pareto-optimal solutions. The evolutionary algorithm would then resemble the optimized dynamic programming algorithm.

12.7 Implementation Notes

We have seen several generic approaches to optimization that are applicable to a wide variety of problems. When you face a new application, you are therefore likely to have the choice between more approaches than you can realistically implement. In a commercial environment, you may even have to home in on a single approach quickly. Here are some rules of thumb that may help:

- study the problem, relate it to problems you are familiar with, and search for it on the web.
- look for approaches that have worked on related problems.
- consider black box solvers.
- if problem instances are small, systematic search or dynamic programming may allow you to find optimal solutions.
- if none of the above looks promising, implement a simple prototype solver using a greedy approach or some other simple and fast heuristic; the prototype helps you to understand the problem and might be useful as a component of a more sophisticated algorithm.
- develop a local search algorithm. Focus on a good representation for solutions and how to incorporate application specific knowledge into the searcher. If you have a promising idea for a mating operator, you can also consider evolutionary algorithms. Use randomization and restarts to make the results more robust.

There are many implementations of linear programming solvers. Since a good implementation is *very* complicated, you should use one of these packages except in very special circumstances. The Wikipedia page on linear programming is a good starting point. Some systems for linear programming also support integer linear programming.

There are also many frameworks that simplify implementing local search or evolutionary algorithms. Since these algorithms are fairly simple, using the frameworks is not as widespread as for linear programming. Nevertheless, the implementations might have non-trivial built-in algorithms for dynamic setting of search parameters and they might support parallel processing. [kennen wir irgendwelche wirklich empfehlenswerte Systeme? CILib? `http://eodev.sourceforge.net/`?] ⟹

12.8 Historical Notes and Further Findings

We have only scratched the surface of (integer) linear programming. Implementing solvers, clever modeling of problems, and handling huge input instances have led to thousands of scientific papers. In the late 1940s, Dantzig invented the simplex algorithm [46]. Although this algorithm works well in practice, some of its variants take exponential time in the worst case. It is a famous open problem whether some variant runs in polynomial time in the worst case. It is known though that even slightly perturbing the coefficients of the constraints leads to polynomial expected execution time [174]. Sometimes, even problem instances with an exponential number of constraints or variables can be solved efficiently. The trick is to handle explicitly only constraints that may be violated and variables that may be non-zero in an optimal solution. This works, if we can efficiently find violated constraints or possibly non-zero variables and if the total number of generated constraints and variables remains small. Khachiyan [107] and Karmakar [103] found polynomial time algorithms for linear programming. There are many good text books on linear programming, e.g. [24, 139, 162, 59, 187, 73].

Another interesting black box solver is *constraint programming*, cf. [117, 89]. We hinted at the technique in Exercise 227. We are again dealing with variables and constraints. However, now the variables come from discrete sets (usually small finite sets). Constraints come in a much wider variety. There are equalities and inequalities possibly involving arithmetic expressions but also higher-level constraints. For example, $\mathit{allDifferent}(x_1, \ldots, x_k)$ requires that $x_1, \ldots, x_k$ all receive different values. Constraint programs are solved using cleverly pruned systematic search. Constraint programming is more flexible than linear programming but restricted to smaller problem instances. Wikipedia is a good starting point for learning more about constraint programming.

[was passiert mit Material in Summary?] ⟸

A

Appendix

[section on recurrences and inequalities] ⟸

A.1 General Mathematical Notation

$\{e_0, \ldots, e_{n-1}\}$: Set containing elements e_0,. . . ,e_{n-1}.

$\{e : P(e)\}$: Set of all elements fulfilling predicate P.

$\langle e_0, \ldots, e_{n-1}\rangle$: Sequence consisting of elements e_0,. . . ,e_{n-1}.

$\langle e \in S : P(e)\rangle$: subsequence of all elements of sequence S fulfilling predicate P.[ps:reinserted since it is used in three chapters] ⟸

$|x|$: The absolute value of x.

$\lfloor x \rfloor$: The largest integer $\leq x$.

$\lceil x \rceil$: The smallest integer $\geq x$.

$[a, b] := \{x \in \mathbb{R} : a \leq x \leq b\}$.[check halboffene Intervalle?] ⟸

$i..j$: Abbreviation for $\{i, i+1, \ldots, j\}$.

A^B: when A and B are sets this is the set of all functions mapping B to A.

$A \times B$: The set of pairs (a, b) with $a \in A$ and $b \in B$.

$(f_s)_{s \in S}$: An alternative way to define a function f on S. The accompanying text specifies the range of the function. So "let $d : V \to \mathbb{R}$ be a function on the vertices V of a graph" is equivalent to "let $(d_v)_{v \in V}$ be a real-valued function on the vertices V of a graph". [ps: this complicated and rather specialized notation is only used very locally in optimization (?). Define there and drop here?] ⟸

$\perp$**:** An undefined value.

$(-)\infty$**:** (Minus) infinity.

$\forall x : P(x)$**:** For *all* values of x the proposition $P(x)$ is true.

$\exists x : P(x)$**:** There *exists* a value of x such that the proposition $P(x)$ is true.

$\mathbb{N}$**:** Non-negative integers, $\mathbb{N} = \{0, 1, 2, \ldots\}$

$\mathbb{N}_+$**:** Positive integers, $\mathbb{N}_+ = \{1, 2, \ldots\}$.

$\mathbb{Z}$**:** Integers

$\mathbb{R}$**:** Real numbers

$\mathbb{Q}$**:** Rational numbers

|**,** &**,** «**,** »**,** $\oplus$**:** Bit-wise 'or', 'and', right-shift, left-shift, and exclusive-or respectively.

$\sum_{i=1}^{n} a_i = \sum_{1 \leq i \leq n} a_i = \sum_{i \in \{1,\ldots,n\}} a_i \ := a_1 + a_2 + \cdots + a_n$

$\prod_{i=1}^{n} a_i = \prod_{1 \leq i \leq n} \prod_{i \in \{1,\ldots,n\}} a_i \ := a_1 \cdot a_2 \cdots a_n$

$n! \ := \prod_{i=1}^{n} i$ — the *factorial* of n.

div**:** Integer division. $c = m \,\mathrm{div}\, n$ is the largest non-negative integer with $cn \leq m$.

mod**:** Modular arithmetic, $m \bmod n = m - n(m \,\mathrm{div}\, n)$.

$a \equiv b(\mathrm{mod} m)$**:** a and b are congruent modulo m, i.e., $a + im = b$ for some integer i.

$\prec$**:** Some ordering relation. In Section 9.2 it denotes the order in which nodes are marked during depth-first search.

$\Longrightarrow$1**,** 0**:** The boolean values true and false[check with intro].

antisymmetric: A relation $\sim$ is *antisymmetric* if for all a and b, $a \sim b$ and $b \sim a$ implies $a = b$.

concave: A function f is concave on an interval $[a, b]$ if
$\forall x, y \in [a, b], t \in [0, 1] : f(tx + (1-t)y) \geq tf(x) + (1-t)f(y)$.

convex: A function f is convex on an interval $[a, b]$ if
$\forall x, y \in [a, b], t \in [0, 1] : f(tx + (1-t)y) \leq tf(x) + (1-t)f(y)$.

equivalence relation: a transitive, reflexive, symmetric relation.

field: A set of elements that support addition, subtraction, multiplication, and division by non-zero elements. Addition and multiplication are associative, commutative, and have neutral elements analogous to zero and one for the real numbers. The prime examples are $\mathbb{R}$, the real numbers, $\mathbb{Q}$, the rational numbers $\mathbb{Q}$, and $\mathbb{Z}_p$, the integers modulo a prime p.

$H_n := \sum_{i=1}^{n} 1/i$ the n-th *harmonic number*. See also Equation (A.12).

iff: Abbreviation for "if and only if".

lexicographic order: The most common way to extend a total order on a set of elements to tuples, strings, or sequences of these elements. We have $\langle a_1, a_2, \ldots, a_k\rangle < \langle b_1, b_2, \ldots, b_k\rangle$ if and only if $a_1 < b_1$ or $a_1 = b_1$ and $\langle a_2, \ldots, a_k\rangle < \langle b_2, \ldots, b_k\rangle$

linear order: See total order.

$\log x$**:** The logarithm base two of x, $\log_2 x$.

median: An element with rank $\lceil n/2\rceil$ among n elements.

multiplicative inverse: If an object x is multiplied with a *multiplicative inverse* x^{-1} of x, we obtain $x \cdot x^{-1} = 1$ — the neutral element of multiplication. In particular, in a *field* every element but zero (the neutral element of addition) has a unique multiplicative inverse. [ps: removed Ω for a sample space. This was used only locally anyway.] $\Longleftarrow$

$\mathcal{O}(f(n)) := \{g(n) : \exists c > 0 : \exists n_0 \in \mathbb{N}_+ : \forall n \geq n_0 : g(n) \leq c \cdot f(n)\}$. (see

$\Omega(f(n)) := \{g(n) : \exists c > 0 : \exists n_0 \in \mathbb{N}_+ : \forall n \geq n_0 : g(n) \geq c \cdot f(n)\}$. also

$\Theta(f(n)) := \mathcal{O}(f(n)) \cap \Omega(f(n))$. Section

$o(f(n)) := \{g(n) : \forall c > 0 : \exists n_0 \in \mathbb{N}_+ : \forall n \geq n_0 : g(n) \leq c \cdot f(n)\}$. 2.1

$\omega(f(n)) := \{g(n) : \forall c > 0 : \exists n_0 \in \mathbb{N}_+ : \forall n \geq n_0 : g(n) \geq c \cdot f(n)\}$.)

prime number: An integer n, $n \geq 2$ is a prime iff there are no integers $a, b > 1$ such that $n = a \cdot b$.

rank: A one-to-one mapping $r : S \to 1..n$ is a ranking function for the elements of a set $S = \{e_1, \ldots, e_n\}$ if $r(x) < r(y)$ whenever $x < y$.

reflexive: A relation $\sim \subseteq A \times A$ is reflexive if $\forall a \in A : (a, a) \in R$.

relation: A set of pairs R. Often we write relations as operators, e.g., if $\sim$ is relation, $a \sim b$ means $(a, b) \in \sim$.

symmetric relation: A relation $\sim$ is *symmetric* if for all a and b, $a \sim b$ implies $b \sim a$.

total order: A reflexive, transitive, antisymmetric relation.

transitive: A relation $\sim$ is *transitive* if for all a, b, c, $a \sim b$ and $b \sim c$ imply $a \sim c$.

A.2 Basic Probability Theory

⟹ [ps: macrofied the terms SampleSpace and Sample. I would like to avoid Ω to avoid collisions with asymptotics. Moreover this stuff is used only here.] Probability theory rests on the concept of a *sample space* $\mathcal{S}$. For example, to describe the role of two dice, we would use the 36 element sample space $\{1,\ldots,6\}\times\{1,\ldots,6\}$, i.e., the elements of the sample space are the pairs (x,y) with $1 \le x,y \le 6$ and $x,y \in \mathbb{N}$. Generally, a sample space is any set. In this book, all sample spaces are finite. In a *(uniform) random experiment*, any element of $\mathcal{S}$ is chosen with the elementary *probability* $p = 1/|\mathcal{S}|$. More generally, an element $s \in \mathcal{S}$ is chosen with probability p_s where $\sum_{s\in\mathcal{S}} p_s = 1$. In this book, we will almost exclusively use uniform probabilities; then $p_s = p = 1/|\mathcal{S}|$. Subsets $\mathcal{E}$ of the sample space are called *events*. The probability of an *event* $\mathcal{E} \subseteq \mathcal{S}$ is the sum of the probabilities of its elements, i.e, $\mathrm{prob}(\mathcal{E}) = |\mathcal{E}|/|\mathcal{S}|$. So the probability of the event $\{(x,y) : x+y=7\} = \{(1,6),(2,5),\ldots,(6,1)\}$ is equal to $6/36 = 1/6$ and the probability of the event $\{(x,y) : x+y \ge 8\}$ is equal to $15/36 = 5/12$.

A *random variable* is a mapping from the sample space to the real numbers. Random variables are usually denoted by capital letters to distinguish them from plain values. A random variable is a familiar concept under a new name. A random variable X is a function from $\mathcal{S}$ to $\mathbb{R}$. For example, the random variable X could give the number shown by the first dice, the random variable Y could give the number shown by the second dice, and the random variable S could give the sum of the two numbers. Formally, if $(x,y) \in \mathcal{S}$ then $X((x,y)) = x$, $Y((x,y)) = y$, and $S((x,y)) = x+y = X((x,y)) + Y((x,y))$.

We can define new random variables as expressions involving other random variables and ordinary values. For example, if X and Y are random variables, then $(X+Y)(s) = X(s)+Y(s)$, $(X\cdot Y)(s) = X(s)\cdot Y(s)$, $(X+3)(s) = X(s)+3$.

Events are often specified by predicates involving random variables. For example, $X \le 2$ denotes the event $\{(1,y),(2,y) : 1 \le y \le 6\}$ and hence $\mathrm{prob}(X \le 2) = 1/3$. Similarly, $\mathrm{prob}(X+Y=11) = \mathrm{prob}(\{(5,6),(6,5)\}) = 1/18$.

Indicator random variables are random variables that only take the values zero and one. Indicator variables are an extremely useful tool for the probabilistic analysis of algorithms because they allow us to encode the behavior of complex algorithms into simple mathematical objects. We frequently use the letters I and J for indicator variables.

The *expected value* of a random variable $Z : \mathcal{S} \to \mathbb{R}$ is

$$\mathrm{E}[Z] = \sum_{s\in\mathcal{S}} p_s \cdot Z(s) = \sum_{z\in\mathbb{R}} z \cdot \mathrm{prob}(Z=z) \enspace , \tag{A.1}$$

i.e., every sample s contributes the value of Z at s times its probability. Alternatively, we group all s with $Z(s) = z$ into the event $Z = z$ and then sum over the $z \in \mathbb{R}$.

In our example, $\mathrm{E}[X] = \frac{1+2+3+4+5+6}{6} = \frac{21}{6} = 3.5$, i.e., the expected value of the first dice is 3.5. Of course, the expected value of the second dice is also 3.5. For an indicator random variable I we have

$$\mathrm{E}[I] = 0 \cdot \mathrm{prob}(I = 0) + 1 \cdot \mathrm{prob}(I = 1) = \mathrm{prob}(I = 1) \ .$$

Often we are interested in the expectation of a random variable that is defined in terms of other random variables. This is easy for sums due to the so-called *linearity of expectations* of random variables: For any two random variables X and Y,

$$\mathrm{E}[X + Y] = \mathrm{E}[X] + \mathrm{E}[Y] \ . \tag{A.2}$$

The equation is easy to prove and extremely useful. Let us prove it. It amounts essentially to an application of the distributive law of arithmetic. We have

$$\begin{aligned}
\mathrm{E}[X + Y] &= \sum_{s \in \mathcal{S}} p_s \cdot (X(s) + Y(s)) \\
&= \sum_{s \in \mathcal{S}} p_s \cdot X(s) + \sum_{s \in \mathcal{S}} p_s \cdot Y(s) \\
&= \mathrm{E}[X] + \mathrm{E}[Y] \ .
\end{aligned}$$

As our first application, let us compute the expected sum of two dices. We have

$$\mathrm{E}[S] = \mathrm{E}[X + Y] = \mathrm{E}[X] + \mathrm{E}[Y] = 3.5 + 3.5 = 7 \ .$$

Observe, that we obtain the result with almost no computation. Without knowing about linearity of expectations, we would have to go through a tedious calculation:

$$\begin{aligned}
\mathrm{E}[S] &= 2 \cdot \frac{1}{36} + 3 \cdot \frac{2}{36} + 4 \cdot \frac{3}{36} + 5 \cdot \frac{4}{36} + 6 \cdot \frac{5}{36} + 7 \cdot \frac{6}{36} \\
&\qquad + 8 \cdot \frac{5}{36} + 9 \cdot \frac{4}{36} + \ldots + 12 \cdot \frac{1}{36} \\
&= \frac{2 \cdot 1 + 3 \cdot 2 + 4 \cdot 3 + 5 \cdot 4 + 6 \cdot 5 + 7 \cdot 6 + 8 \cdot 5 + \ldots + 12 \cdot 1}{36} = 7 \ .
\end{aligned}$$

Exercise 232. What is the expected sum of three dices?

We will give another example with a more complex sample space. The sample space consists of all $n!$ permutations of the numbers 1 to n. We are interested in the expected number of left-to-right maxima in a random permutation. A left-to-right maximum in a sequence is an element which is larger than all preceding elements. So $(1, 2, 4, 3)$ has three left-to-right-maxima and $(3, 1, 2, 4)$ has two left-to-right-maxima. For a permutation π of the integers 1 to n, let $M_n(\pi)$ be the number of left-to-right-maxima. What is $\mathrm{E}[M_n]$? For small n, is easy to determine $\mathrm{E}[M_n]$ by direct calculation. For $n = 1$, there is only one permutation, namely (1) and it has one maximum. So $\mathrm{E}[M_1] = 1$. For $n = 2$, there are two permutations, namely $(1, 2)$ and $(2, 1)$. The former has two maxima and the latter has one maximum. So $\mathrm{E}[M_2] = 1.5$.

Exercise 233. Determine $\mathrm{E}[M_3]$ and $\mathrm{E}[M_4]$.

We now show how to determine $\mathrm{E}[M_n]$. We write M_n as a sum of indicator variables I_1 to I_n, i.e., $M_n = I_1 + \ldots + I_n$ where I_k is equal to one for a permutation π if the k-th element of π is a left-to-right-maximum. For example, $I_3((3,1,2,4)) = 0$ and $I_4((3,1,2,4)) = 1$. We have

$$\begin{aligned}\mathrm{E}[M_n] &= \mathrm{E}[I_1 + I_2 + \ldots + I_n] \\ &= \mathrm{E}[I_1] + \mathrm{E}[I_2] + \ldots + \mathrm{E}[I_n] \\ &= \mathrm{prob}(I_1 = 1) + \mathrm{prob}(I_2 = 1) + \ldots + \mathrm{prob}(I_n = 1) \ ,\end{aligned}$$

where the second equality is linearity of expectations and the third equality follows from the I_k's being indicator variables. It remains to determine the probability that $I_k = 1$. The k-th element of a random permutation is a left-to-right maximum with probability $1/k$ because this is the case if and only if the k-th element is the largest of the first k elements. Since every permutation of the first k elements is equally likely, this probability is $1/k$. Thus $\mathrm{prob}(I_k = 1) = 1/k$ and hence

$$\mathrm{E}[M_n] = \sum_{1 \le k \le n} \mathrm{prob}(I_k = 1) = \sum_{1 \le k \le n} 1/k = H_n \ ,$$

where $H_n = \sum_{1 \le k \le n} 1/k$ is the so-called n-th Harmonic number, see Equation (A.12). So $\mathrm{E}[M_4] = 1 + 1/2 + 1/3 + 1/4 = (12 + 6 + 4 + 3)/12 = 25/12$.

Products of random variables behave differently. In general, we have $\mathrm{E}[X \cdot Y] \neq \mathrm{E}[X] \cdot \mathrm{E}[Y]$. There is one important exception: if X and Y are *independent*, equality holds. Random variables $X_1, \ldots, X_k$ are independent if and only if

$$\forall x_1, \ldots, x_k : \mathrm{prob}(X_1 = x_1 \wedge \cdots \wedge X_k = x_k) = \prod_{1 \le i \le k} \mathrm{prob}(X_i = x_i) \qquad \text{(A.3)}$$

As an example, when we role two dice, the value of the first dice and the value of the second dice are independent random variables. However, the value of the first dice and the sum of the two dices are not independent random variables.

Exercise 234. Let I and J be independent indicator variables and let $X = (I + J) \bmod 2$, i.e., X is one iff I and J are different. Show that I and X are independent, but that I, J, and X are dependent.

Assume now that X and Y are independent. Then

$$\begin{aligned}
\mathrm{E}[X]\cdot\mathrm{E}[Y] &= (\sum_x x\cdot\mathrm{prob}(X=x))\cdot(\sum_y y\cdot\mathrm{prob}(X=y))\\
&= \sum_{x,y} x\cdot y\cdot\mathrm{prob}(X=x)\cdot\mathrm{prob}(X=y)\\
&= \sum_{x,y} x\cdot y\cdot\mathrm{prob}(X=x\wedge Y=y)\\
&= \sum_z \sum_{x,y\text{ with }z=x\cdot y} z\cdot\mathrm{prob}(X=x\wedge Y=y)\\
&= \sum_z z\cdot \sum_{x,y\text{ with }z=x\cdot y} \mathrm{prob}(X=x\wedge Y=y)\\
&= \sum_z z\cdot\mathrm{prob}(X\cdot Y=z)\\
&= \mathrm{E}[X\cdot Y]\ .
\end{aligned}$$

How likely is it that a random variable deviates substantially from its expected value? The so-called *Tschebyscheff inequality* gives a useful bound. Let X be a non-negative random variable and let c be any constant. Then

$$\mathrm{prob}(X\geq c\cdot\mathrm{E}[X])\leq\frac{1}{c}\ . \tag{A.4}$$

The proof is simple. We have

$$\begin{aligned}
\mathrm{E}[X] &= \sum_{z\in\mathbb{R}} z\cdot\mathrm{prob}(X=z)\\
&\geq \sum_{z\geq c\cdot\mathrm{E}[X]} z\cdot\mathrm{prob}(X=z)\\
&\geq c\cdot\mathrm{E}[X]\cdot\mathrm{prob}(X\geq c\cdot\mathrm{E}[X])\ ,
\end{aligned}$$

where the first inequality follows from the fact that we sum over a subset of the possible values and X is non-negative and the second inequality follows from the fact that the sum in the second line ranges only over z with $z\geq c\mathrm{E}[X]$.

Much tighter bounds are possible for special cases of random variables. The following situation will come up several times. We have a sum $X=X_1+\cdots+X_n$ of n independent(!!) indicator random variables $X_1,\ldots,X_n$ and want to bound the probability that X deviates substantially from its expected value. In this situation, the following variant of the so-called *Chernoff bound* is useful. For any $\epsilon>0$, we have:

$$\mathrm{prob}(X<(1-\epsilon)\mathrm{E}[X])\leq e^{-\epsilon^2\mathrm{E}[X]/2} \tag{A.5}$$

$$\mathrm{prob}(X>(1+\epsilon)\mathrm{E}[X])\leq\left(\frac{e^{\epsilon}}{(1+\epsilon)^{(1+\epsilon)}}\right)^{\mathrm{E}[X]}\ . \tag{A.6}$$

A bound of the form above is also called a *tail bound* because it estimates the "tail of the probability" distribution, i.e., the part for which X is deviates considerably from its expected value.

Let us see an example. If we role n dices and let X_i denote the value of the i-th dice, then $X = X_1 + \cdots + X_n$ is the sum of the n dices. We know already that $\mathrm{E}[X] = 7n/2$. The bound above tells us that $\mathrm{prob}(X \leq (1-\epsilon)7n/2) \leq e^{-\epsilon^2 7n/4}$. In particular, for $\epsilon = 0.1$ we have $\mathrm{prob}(X \leq 0.9 \cdot 7n/2) \leq e^{-0.01 \cdot 7n/4}$. So for $n = 1000$, the expected sum is 3500 and the probability that the sum is less than 3150 is smaller than e^{-17}, a very small number.

Exercise 235. Estimate the probability that X is larger than 3850.

If the indicator random variables are independent and identically distributed with $\mathrm{prob}(X_i = 1) = p$, X is *binomially distributed*, i.e.,

$$\mathrm{prob}(X = i) = \binom{n}{i} p^i (1-p)^{(n-i)} \quad . \tag{A.7}$$

A.3 Useful Formulae

We will first list some useful formulae and then prove some of them.

$$\left(\frac{n}{e}\right)^n \leq n! \leq n^n \tag{A.8}$$

$$\text{Stirling's approximation of the factorial: } n! = \left(1 + \mathcal{O}\left(\frac{1}{n}\right)\right) \sqrt{2\pi n} \left(\frac{n}{e}\right)^n \tag{A.9}$$

$$\binom{n}{k} \leq \left(\frac{n \cdot e}{k}\right)^k \tag{A.10}$$

$$\sum_{i=1}^{n} i = \frac{n(n+1)}{2} \tag{A.11}$$

$$\text{Harmonic Numbers: } \ln n \leq H_n = \sum_{i=1}^{n} \frac{1}{i} \leq \ln n + 1 \tag{A.12}$$

$$\sum_{i=0}^{n-1} q^i = \frac{1-q^n}{1-q} \quad \text{for } q \neq 1 \text{ and } \quad \sum_{i \geq 0} q^i = \frac{1}{1-q} \quad \text{for } 0 \leq q < 1 \tag{A.13}$$

$$\sum_{i \geq 0} 2^{-i} = 2 \quad \text{and} \quad \sum_{i \geq 0} i \cdot 2^{-i} = \sum_{i \geq 1} i \cdot 2^{-i} = 2 \tag{A.14}$$

$\Longrightarrow$ [ps todo: schÃűnere Ausrichtung der benamsten Gleichungen]

$$\text{Jensen's inequality:} \sum_{i=1}^{n} f(x_i) \le n \cdot f\left(\frac{\sum_{i=1}^{n} x_i}{n}\right) \tag{A.15}$$

for any concave function f. Similarly, for any convex function f,

$$\sum_{i=1}^{n} f(x_i) \ \ge n \cdot f\left(\frac{\sum_{i=1}^{n} x_i}{n}\right) \quad . \tag{A.16}$$

Proofs:

For Equation (A.8), we first observe $n! = n(n-1)\cdots 1 \le n^n$. Also, for all $i \ge 2$, $\ln i \ge \int_{i-1}^{i} \ln x \, dx$ and therefore

$$\ln n! = \sum_{2 \le i \le n} \ln i \ge \int_1^n \ln x \, dx = \Big[x(\ln x - 1)\Big]_{x=1}^{x=n} \ge n(\ln n - 1) \quad .$$

Thus

$$n! \ge e^{n(\ln n - 1)} = (e^{\ln n - 1})^n = (\frac{n}{e})^n \ .$$

Equation (A.10) follows almost immediately from Equation (A.8). We have

$$\binom{n}{k} = n(n-1)\cdots(n-k+1)/k! \le n^k/(k/e)^k = ((n \cdot e)/k)^k \ .$$

Equation (A.11) can be computed by a simple trick.

$$\begin{aligned} 1 + 2 + \ldots + n &= \frac{1}{2}\left((1 + 2 + \ldots + n - 1 + n) + (n + n - 1 + \ldots + 2 + 1)\right) \\ &= \frac{1}{2}\left((n+1) + (2 + n - 1) + \ldots + (n - 1 + 2) + (n+1)\right) \\ &= n(n+1)/2 \ . \end{aligned}$$

The sums of higher powers are estimated easily; exact summation formulae are also available. For example, $\int_{i-1}^{i} x^2 \, dx \le i^2 \le \int_i^{i+1} x^2 \, dx$ and hence

$$\sum_{1 \le i \le n} i^2 \le \int_1^{n+1} x^2 \, dx = \left[\frac{x^3}{3}\right]_{x=1}^{x=n+1} = \frac{(n+1)^3 - 1}{3}$$

and

$$\sum_{1 \le i \le n} i^2 \ge \int_0^n x^2 \, dx = \left[\frac{x^3}{3}\right]_{x=0}^{x=n} = \frac{n^3}{3} \ .$$

For Equation (A.12), we also use estimation by integral. We have $\int_{i-1}^{i} 1/x\,dx \geq 1/i \geq \int_{i}^{i+1} 1/x\,dx$ and hence

$$\ln n \leq \int_1^n \frac{1}{x}\,dx \leq \sum_{1 \leq i \leq n} \frac{1}{i} \leq 1 + \int_1^n \frac{1}{x}\,dx = 1 + \ln n\ .$$

Equation (A.13) follows from

$$(1-q) \cdot \sum_{0 \leq i \leq n-1} q^i = \sum_{0 \leq i \leq n-1} q^i - \sum_{1 \leq i \leq n} q^i = 1 - q^n\ \ .$$

Letting n pass to infinity yields $\sum_{i \geq 0} q^i = 1/(1-q)$ for $0 \leq q < 1$. For $q = 1/2$, we obtain $\sum_{i \geq 0} 2^{-i} = 2$. Also,

$$\begin{aligned}\sum_{i \geq 1} i \cdot 2^{-i} &= \sum_{i \geq 1} 2^{-i} + \sum_{i \geq 2} 2^{-i} + \sum_{i \geq 3} 2^{-i} + \ldots \\ &= (1 + 1/2 + 1/4 + 1/8 + \ldots) \cdot \sum_{i \geq 1} 2^{-i} \\ &= 2 \cdot 1 = 2\ .\end{aligned}$$

For the first equality observe that the term 2^{-i} occurs exactly in the first i sums of the right-hand side of the first equality.

Equation (A.16) can be shown by induction on n. For $n = 1$, there is nothing to show. So assume $n \geq 2$. Let $x^* = \sum_{1 \leq i \leq n} x_i/n$ and $\bar{x} = \sum_{1 \leq i \leq n-1} x_i/(n-1)$. Then $x^* = ((n-1)\bar{x} + x_n)/n$ and hence

$$\begin{aligned}\sum_{1 \leq i \leq n} f(x_i) &= f(x_n) + \sum_{1 \leq i \leq n-1} f(x_i) \\ &\leq f(x_n) + (n-1) \cdot f(\bar{x}) = n \cdot \left(\frac{1}{n} \cdot f(x_n) + \frac{n-1}{n} \cdot f(\bar{x})\right) \\ &\leq n \cdot f(x^*)\ ,\end{aligned}$$

where the first inequality uses the induction hypothesis and the second inequality uses the definition of concavity with $x = x_n$, $y = \bar{x}$ and $t = 1/n$. The extension to convex functions is immediate, since convexity of f implies concavity of $-f$.

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