Chapter 6

Recurrence Relations[1]

6.1 SOME EXAMPLES

At the beginning of Section 5.1, we saw that we frequently want to count a quantity a_k that depends on an input or a parameter k. We then studied the sequence of unknown values, $a_0, a_1, a_2, \ldots, a_k, \ldots$. We shall see how to reduce computation of the kth or the $(k+1)$st member of such a sequence to earlier members of the sequence. In this way we can reduce a bigger problem to a smaller one or to one solved earlier. In Section 3.4 and in Example 5.14, we did much the same thing by giving reduction theorems, which reduced a complicated computation to simpler ones or ones made earlier. Having seen how to reduce computation of later terms of a sequence to earlier terms, we discuss several methods for finding general formulas for the kth term of an unknown sequence. The ideas and methods we present will have a wide variety of applications.

6.1.1 Some Simple Recurrences

Example 6.1 The Grains of Wheat According to Gamow [1954], the following is the story of King Shirham of India. The King wanted to reward his Grand Vizier, Sissa Ben Dahir, for inventing the game of chess. The Vizier made a modest request: Give me one grain of wheat for the first square on a chess board, two grains for the second square, four for the third square, eight for the fourth square, and so on until all the squares are covered. The King was delighted at the modesty of his Vizier's request, and granted it immediately. Did the King do a very wise thing? To answer this question, let s_k be the number of grains of wheat required for the first k squares and t_k be the number of grains for the kth square. We have

$$t_{k+1} = 2t_k. \tag{6.1}$$

[1] If Chapter 5 has been omitted, Sections 6.3 and 6.4 should be omitted. Chapters 5 and 6 are the only chapters that assume calculus except for the sake of "mathematical maturity." The only calculus used in Chapter 6 except in Sections 6.3 and 6.4 is elementary knowledge about infinite sequences; even here, the concept of limit is used in only a few applications, and these can be omitted.

Equation (6.1) is an example of a *recurrence relation*, a formula reducing later values of a sequence of numbers to earlier ones. Let us see how we can use the recurrence formula to get a general expression for t_k. We know that $t_1 = 1$. This is given to us, and is called an *initial condition*. We know that

$$\begin{aligned} t_2 &= 2t_1 \\ t_3 &= 2t_2 = 2^2 t_1 \\ t_4 &= 2t_3 = 2^2 t_2 = 2^3 t_1, \end{aligned}$$

and in general

$$t_k = 2t_{k-1} = \cdots = 2^{k-1} t_1.$$

Using the initial condition, we have

$$t_k = 2^{k-1} \tag{6.2}$$

for all k. We have solved the recurrence (6.1) by *iteration* or repeated use of the recurrence. Note that a recurrence like (6.1) will in general have many *solutions*, that is, sequences which satisfy it. However, once sufficiently many initial conditions are specified, there will be a unique solution. Here the sequence $1, 2, 4, 8, \ldots$ is the unique solution given the initial condition. However, if the initial condition is disregarded, any multiple of this sequence is a solution, as, for instance, $3, 6, 12, 24, \ldots$ or $5, 10, 20, 40, \ldots$.

We are really interested in s_k. We have

$$s_{k+1} = s_k + t_{k+1}, \tag{6.3}$$

another form of recurrence formula that relates later values of s to earlier values of s and to values of t already calculated. We can reduce (6.3) to a recurrence for s_k alone by using (6.2). This gives us

$$s_{k+1} = s_k + 2^k. \tag{6.4}$$

Let us again use iteration to solve the recurrence relation (6.4) for s_k for all k. We have

$$\begin{aligned} s_2 &= s_1 + 2 \\ s_3 &= s_2 + 2^2 = s_1 + 2 + 2^2, \end{aligned}$$

and in general

$$s_k = s_{k-1} + 2^{k-1} = \cdots = s_1 + 2 + 2^2 + \cdots + 2^{k-1}.$$

Since we have the initial condition $s_1 = 1$, we obtain

$$s_k = 1 + 2 + 2^2 + \cdots + 2^{k-1}.$$

This expression can be simplified if we use the following well-known identity, which we have already encountered in Chapter 5:

$$1 + x + x^2 + \cdots + x^p = \frac{1 - x^{p+1}}{1 - x}.$$

Using this identity with $x = 2$ and $p = k - 1$, we have

$$s_k = \frac{1 - 2^k}{1 - 2} = 2^k - 1.$$

Now there are 64 squares on a chess board. Hence, the number of grains of wheat the Vizier asked for is given by $2^{64} - 1$, which is

$$18{,}446{,}744{,}073{,}709{,}551{,}615,$$

a very large number indeed![2] ■

Example 6.2 Computational Complexity One major use of recurrences in computer science is in the computation of the complexity $f(n)$ of an algorithm with input of size n (see Section 2.4). Often, computation of the complexity $f(n+1)$ is reduced to knowledge of the complexities $f(n)$, $f(n-1)$, and so on. As a trivial example, let us consider the following algorithm for summing the first n entries of a sequence or an array A.

Algorithm 6.1: Summing the First n Entries of a Sequence or an Array

Input: A sequence or an array A and a number n.
Output: The sum $A(1) + A(2) + \cdots + A(n)$.

Step 1. Set $i = 1$.

Step 2. Set $T = A(1)$.

Step 3. If $i = n$, stop and output T. Otherwise, set $i = i + 1$ and go to step 4.

Step 4. Set $T = T + A(i)$ and return to step 3.

If $f(n)$ is the number of additions performed in summing the first n entries of A, we have the recurrence

$$f(n) = f(n-1) + 1. \tag{6.5}$$

Also, we have the initial condition $f(1) = 0$. Thus, by iteration, we have

$$f(n) = f(n-1) + 1 = f(n-2) + 1 + 1 = \cdots = f(1) + n - 1 = n - 1.$$ ■

Example 6.3 Simple and Compound Interest Suppose that a sum of money S_0 is deposited in a bank at *interest rate* r per interest period (say, per year), that is, at $100r$ percent. If the interest is *simple*, after every interest period a fraction r

[2] All of the sequences from this chapter can be found at the *On-Line Encyclopedia of Integer Sequences* (Sloane [2003]). This is a database of over 90,000 sequences. The entry for each sequence gives the beginning terms of the sequence, its name or description, references, formulas, and so on.

of the initial deposit S_0 is credited to the account. If S_k is the amount on deposit after k periods, we have the recurrence

$$S_{k+1} = S_k + rS_0. \tag{6.6}$$

By iteration, we find that

$$S_k = S_{k-1} + rS_0 = S_{k-2} + rS_0 + rS_0 = \cdots = S_0 + krS_0,$$

so

$$S_k = S_0(1 + kr).$$

If interest is *compounded* each period, we receive as interest after each period a fraction r of the amount on deposit at the beginning of the period; that is, we have the recurrence

$$S_{k+1} = S_k + rS_k,$$

or

$$S_{k+1} = (1 + r)S_k. \tag{6.7}$$

We find by iteration that

$$S_k = (1 + r)^k S_0.$$

■

Example 6.4 Legitimate Codewords Codewords from the alphabet $\{0, 1, 2, 3\}$ are to be recognized as *legitimate* if and only if they have an even number of 0's. How many legitimate codewords of length k are there? Let a_k be the answer. We derive a recurrence for a_k. (Note that a_k could be computed using the method of generating functions of Chapter 5.) Observe that $4^k - a_k$ is the number of illegitimate k-digit codewords, that is, the k-digit words with an odd number of 0's. Consider a legitimate $(k + 1)$-digit codeword. It starts with 1, 2, or 3, or it starts with 0. In the former case, the last k digits form a legitimate codeword of length k, and in the latter case they form an illegitimate codeword of length k. Thus, by the product and sum rules of Chapter 2,

$$a_{k+1} = 3a_k + 1(4^k - a_k),$$

that is,

$$a_{k+1} = 2a_k + 4^k. \tag{6.8}$$

We have the initial condition $a_1 = 3$. One way to solve the recurrence (6.8) is by the method of iteration. This is analogous to the solution of recurrence (6.4) and is left to the reader. An alternative method is described in Section 6.3. For now, we compute some values of a_k. Note that since $a_1 = 3$, the recurrence gives us

$$a_2 = 2a_1 + 4^1 = 2(3) + 4 = 10$$

and

$$a_3 = 2a_2 + 4^2 = 2(10) + 16 = 36.$$

The reader might wish to check these numbers by writing out the legitimate codewords of lengths 2 and 3. Note how early values of a_k are used to derive later values. We do not need an explicit solution to use a recurrence to calculate unknown numbers. ■

Example 6.5 Duration of Messages Imagine that we transmit messages over a channel using only two signals, a and b. A codeword is any sequence from the alphabet $\{a, b\}$. Now suppose that signal a takes 1 unit of time to transmit and signal b takes 2 units of time to transmit. Let N_t be the number of possible codewords that can be transmitted in exactly t units of time. What is N_t? To answer this question, consider a codeword transmittable in t units of time. It begins either in a or b. If it begins in a, the remainder is any codeword that can be transmitted in $t-1$ units of time. If it begins in b, the remainder is any codeword that can be transmitted in $t-2$ units of time. Thus, by the sum rule, for $t \geq 2$,

$$N_t = N_{t-1} + N_{t-2}. \tag{6.9}$$

This is our first example of a recurrence where a given value depends on more than one previous value. For this recurrence, since the tth term depends on two previous values, we need two initial values, N_1 and N_2. Clearly, $N_1 = 1$ and $N_2 = 2$, the latter since aa and b are the only two sequences that can be transmitted in 2 units of time. We shall solve the recurrence (6.9) in Section 6.2 after we develop some general tools for solving recurrences. Shannon [1956] defines the *capacity* C of the transmission channel as

$$C = \lim_{t \to \infty} \frac{\log_2 N_t}{t}.$$

This is a measure of the capacity of the channel to transmit information. We return to this in Section 6.2.2. ■

Example 6.6 Transposition Average of Permutations Given a permutation π of $\{1, 2, \ldots, n\}$, Jerrum's formula (2.17) calculates the number of transpositions needed to transform the identity permutation into π. If π is chosen at random, what is the expected number of needed transpositions? Or, put another way, what is the average number of transpositions needed to transform the identity permutation into a permutation π of $\{1, 2, \ldots, n\}$?

Suppose that each of the permutations of $\{1, 2, \ldots, n\}$ are equally likely. Let b_n equal the average number of transpositions needed to transform the identity permutation into a permutation of $\{1, 2, \ldots, n\}$. For example, if $n = 2$, there are two permutations of $\{1, 2\}$, namely, 12 and 21. No transpositions are needed to transform the identity into 12, and one transposition is needed to transform it into 21. The average number of transpositions needed is $b_2 = (0 + 1)/2 = 1/2$. To find b_{n+1}, consider any permutation $\pi = \pi_1\pi_2\cdots\pi_n$ of $\{1, 2, \ldots, n\}$ and let π^i for $i = 1, 2, \ldots, n+1$ be $\pi_1\pi_2\cdots\pi_{i-1}(n+1)\pi_i\cdots\pi_n$. [If $i = n+1$, π^i is $\pi_1\pi_2\cdots\pi_n(n+1)$.] Let $a(\pi)$ be the number of transpositions needed to transform the identity into π and $a(\pi^i)$ be the number needed to transform the identity into

π^i. Note that in π^i, $n+1$ is greater than any of the numbers to its right. Therefore, by Jerrum's formula (2.17), $a(\pi^i) = a(\pi) + [n-(i-1)]$, so

$$\begin{aligned}\sum_{i=1}^{n+1} a(\pi^i) &= [(a(\pi)+n) + (a(\pi)+(n-1)) + \cdots + (a(\pi)+0)] \\ &= [(n+1)a(\pi) + n + (n-1) + \cdots + 0] \\ &= [(n+1)a(\pi) + n(n+1)/2],\end{aligned}$$

by the standard formula for the sum of an arithmetic progression. Then

$$\begin{aligned} b_{n+1} &= \frac{\displaystyle\sum_{\pi}\sum_{i=1}^{n+1} a(\pi^i)}{(n+1)!} \\ &= \frac{\displaystyle\sum_{\pi} [(n+1)a(\pi) + n(n+1)/2]}{(n+1)!} \\ &= \frac{\displaystyle\sum_{\pi} a(\pi)}{n!} + \frac{n!\,(n(n+1)/2)}{(n+1)!} \\ &= b_n + \frac{n}{2}.\end{aligned}$$

To solve this recurrence relation, we note that $b_1 = 0$, $b_2 = \frac{1}{2}$, and

$$\begin{aligned} b_3 &= b_2 + \tfrac{2}{2} = \tfrac{1}{2} + \tfrac{2}{2}, \\ b_4 &= b_3 + \tfrac{3}{2} = \tfrac{1}{2} + \tfrac{2}{2} + \tfrac{3}{2}, \\ b_5 &= b_4 + \tfrac{4}{2} = \tfrac{1}{2} + \tfrac{2}{2} + \tfrac{3}{2} + \tfrac{4}{2}.\end{aligned}$$

In general,

$$b_{n+1} = b_n + \frac{n}{2} = \cdots = \frac{1}{2} + \frac{2}{2} + \frac{3}{2} + \cdots + \frac{n}{2} = \frac{1}{2}(1+2+\cdots+n) = \frac{n(n+1)}{4},$$

again using the standard formula for the sum of an arithmetic progression. ■

Example 6.7 Regions in the Plane A line separates the plane into two regions (see Figure 6.1). Two intersecting lines separate the plane into four regions (again see Figure 6.1). Suppose that we have n lines in "general position"; that is, no two are parallel and no three lines intersect in the same point. Into how many regions do these lines divide the plane? To answer this question, let $f(n)$ be the appropriate number of regions. We have already seen that $f(1) = 2$ and $f(2) = 4$. Figure 6.1 also shows that $f(3) = 7$. To determine $f(n)$, we shall derive a recurrence relation.

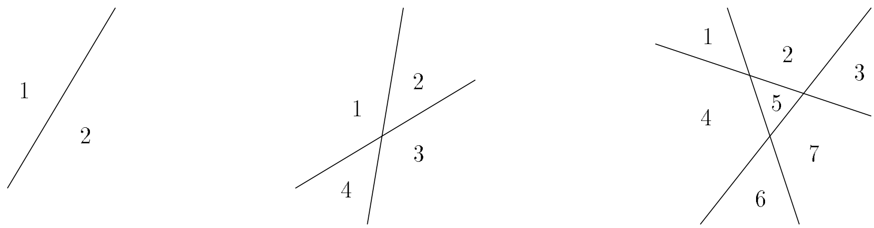

Figure 6.1: Lines dividing the plane into regions.

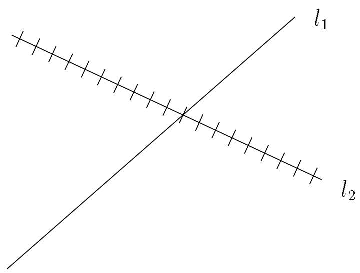

Figure 6.2: Line l_1 divides line l_2 into two segments.

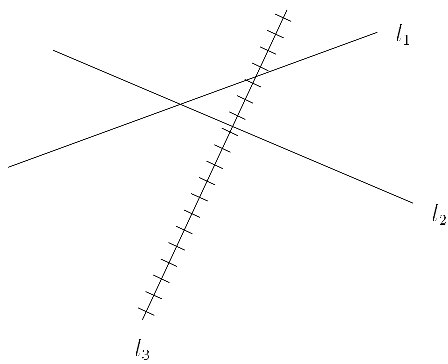

Figure 6.3: Line l_3 is divided by lines l_1 and l_2 into three segments.

Consider a line l_1 as shown in Figure 6.2. Draw a second line l_2. Line l_1 divides line l_2 into two segments, and each segment divides an existing region into two regions. Hence,

$$f(2) = f(1) + 2.$$

Similarly, if we add a third line l_3, this line is divided by l_1 and l_2 into three segments, with each segment splitting an existing region into two parts (see Figure 6.3). Hence,

$$f(3) = f(2) + 3.$$

In general, suppose that we add a line l_{n+1} to already existing lines $l_1, l_2, \ldots, l_n$. The existing lines split l_{n+1} into $n + 1$ segments, each of which splits an existing region into two parts (Figure 6.4). Hence, we have

$$f(n + 1) = f(n) + (n + 1). \tag{6.10}$$

Equation (6.10) gives a recurrence relation that we shall use to solve for $f(n)$. The initial condition is the value of $f(1)$, which is 2. To solve the recurrence relation

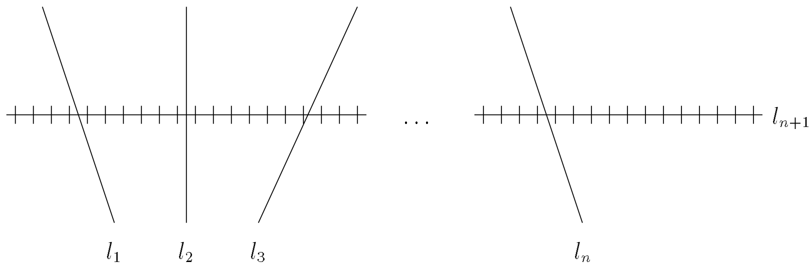

Figure 6.4: Line l_{n+1} is split by lines $l_1, l_2, \ldots, l_n$ into $n+1$ segments.

(6.10), we note that

$$\begin{aligned} f(2) &= f(1) + 2, \\ f(3) &= f(2) + 3 = f(1) + 2 + 3, \\ f(4) &= f(3) + 4 = f(2) + 3 + 4 = f(1) + 2 + 3 + 4, \end{aligned}$$

and in general,

$$f(n) = f(n-1) + n = \cdots = f(1) + 2 + 3 + \cdots + n.$$

Since $f(1) = 2$, we have

$$\begin{aligned} f(n) &= 2 + 2 + 3 + 4 + \cdots + n \\ &= 1 + (1 + 2 + 3 + 4 + \cdots + n) \\ &= 1 + \frac{n(n+1)}{2}, \end{aligned}$$

again using the standard formula for the sum of an arithmetic progression. For example, we have

$$f(4) = 1 + \frac{4 \cdot 5}{2} = 11.$$

■

6.1.2 Fibonacci Numbers and Their Applications

In the year 1202, Leonardo of Pisa, better known as Fibonacci, posed the following problem in his book *Liber Abaci*. Suppose that we study the prolific breeding of rabbits. We start with one pair of adult rabbits (of opposite gender). Assume that each pair of adult rabbits produce one pair of young (of opposite gender) each month. A newborn pair of rabbits become adults in two months, at which time they also produce their first pair of young. Assume that rabbits never die. Let F_k count the number of rabbit pairs present at the beginning of the kth month. Table 6.1 lists for each of several values of k the number of adult pairs, the number of one-month-old young pairs, the number of newborn young pairs, and the total number of rabbit pairs. For example, at the beginning of the second month, there is one newborn rabbit pair. At the beginning of the third month, the newborns from

Table 6.1: Rabbit Breeding

Month k	Number of adult pairs at beginning of month k	Number of one-month-old pairs at beginning of month k	Number of newborn pairs at beginning of month k	Total number of pairs at beginning of month $k = F_k$
1	1	0	0	1
2	1	0	1	2
3	1	1	1	3
4	2	1	2	5
5	3	2	3	8
6	5	3	5	13

the preceding month are one month old, and there is again a newborn pair. At the beginning of the fourth month, the one-month-olds have become adults and given birth to newborns, so there are now two adult pairs and two newborn pairs. The one newborn pair from month 3 has become a one-month-old pair. And so on.

Let us derive a recurrence relation for F_k. Note that the number of rabbit pairs at the beginning of the kth month is given by the number of rabbit pairs at the beginning of the $(k-1)$st month plus the number of newborn pairs at the beginning of the kth month. But the latter number is the same as the number of adult pairs at the beginning of the kth month, which is the same as the number of all rabbit pairs at the beginning of the $(k-2)$th month. (It takes exactly 2 months to become an adult.) Hence, we have for $k \geq 3$,

$$F_k = F_{k-1} + F_{k-2}. \tag{6.11}$$

Note that if we define F_0 to be 1, then (6.11) holds for $k \geq 2$. Observe the similarity of recurrences (6.11) and (6.9). We return to this point in Section 6.2.2. Let us compute several values of F_k using the recurrence (6.11). We already know that

$$F_0 = F_1 = 1.$$

Hence,

$$\begin{aligned} F_2 &= F_1 + F_0 = 2, \\ F_3 &= F_2 + F_1 = 3, \\ F_4 &= F_3 + F_2 = 5, \\ F_5 &= F_4 + F_3 = 8, \\ F_6 &= F_5 + F_4 = 13, \\ F_7 &= F_6 + F_5 = 21, \\ F_8 &= F_7 + F_6 = 34. \end{aligned}$$

In Section 6.2.2 we shall use the recurrence (6.11) to obtain an explicit formula for the number F_k. The sequence of numbers $F_0, F_1, F_2, \ldots$ is called the *Fibonacci* *sequence* and the numbers F_k the *Fibonacci numbers.* These numbers have remarkable properties and arise in a great variety of places. We shall describe some of their properties and applications here.

The *growth rate* at time k of the sequence (F_k) is defined to be

$$G_k = \frac{F_k}{F_{k-1}}.$$

Then we have

$$G_1 = \frac{1}{1} = 1,\ G_2 = \frac{2}{1} = 2,\ G_3 = \frac{3}{2} = 1.5,\ G_4 = \frac{5}{3} = 1.67,\ G_5 = \frac{8}{5} = 1.60,$$

$$G_6 = \frac{13}{8} = 1.625,\ G_7 = \frac{21}{13} = 1.615,\ G_8 = \frac{34}{21} = 1.619,\ \ldots.$$

The numbers G_k seem to be converging to a limit between 1.60 and 1.62. In fact, this limit turns out to be exactly

$$\tau = \frac{1}{2}(1+\sqrt{5}) = 1.618034\ldots.$$

The number τ will arise in the development of a general formula for F_k. [This number is called the *golden ratio* or the *divine proportion.* It is the number with the property that if one divides the line AB at C so that $\tau = AB/AC$, then

$$\frac{AB}{AC} = \frac{AC}{CB}.$$

The rectangle with sides in the ratio $\tau : 1$ is called the *golden rectangle.* A fifteenth-century artist Piero della Francesca wrote a whole book (*De Divina Proportione*) about the applications of τ and the golden rectangle in art, in particular in the work of Leonardo da Vinci. Although much has been made of the golden ratio in the arts, architecture, and aesthetics, it has been argued that many of the golden ratio assertions are either "false or seriously misleading" (Markowsky [1992]).]

Fibonacci numbers have important applications in numerical analysis, in particular in the search for the maximum value of a function $f(x)$ in an interval (a, b). A *Fibonacci search* for the maximum value, performed on a computer, makes use of the Fibonacci numbers to determine where to evaluate the function in getting better and better estimates of the location of the maximum value. When f is concave, this is known to be the best possible search procedure in the sense of minimizing the number of function evaluations for finding the maximum to a desired degree of accuracy. See Adby and Dempster [1974], Hollingdale [1978], or Kiefer [1953].

It is intriguing that Fibonacci numbers appear very frequently in nature. The field of botany that studies the arrangements of leaves around stems, the scales on cones, and so on, is called *phyllotaxis.* Usually, leaves appearing on a given stem or branch point out in different directions. The second leaf is rotated from the first by a certain angle, the third leaf from the second by the same angle, and so on, until some leaf points in the same direction as the first. For example, if the angle of

Table 6.2: Values of n and m for Various Plants

Plant	Angle of rotation	n	m
Elm	180°	2	1
Alder, birch	120°	3	1
Rose	144°	5	2
Cabbage	135°	8	3

Source: Schips [1922]; Batschelet [1971].

rotation is 30°, then the twelfth leaf is the first one pointing in the same direction as the first, since $12 \times 30° = 360°$. If the angle is 144°, then the fifth leaf is the first one pointing in the same direction as the first, for $5 \times 144° = 720°$. Two complete 360° returns have been made before a leaf faces in the same direction as the first. In general, let n count the number of leaves before returning to the same direction as the first, and let m count the number of complete 360° turns that have been made before this leaf is encountered. Table 6.2 shows the values of n and m for various plants. It is a remarkable empirical fact of biology that most frequently both n and m take as values the Fibonacci numbers. There is no good theoretical explanation for this fact.

Coxeter [1969] points out that the Fibonacci numbers also arise in the study of scales on a fir cone, whorls on a pineapple, and so on. These whorls (cells) are arranged in fairly visible diagonal rows. The whorls can be assigned integers in such a way that each diagonal row of whorls forms an arithmetic sequence with common difference (difference between successive numbers) a Fibonacci number. This is shown in Figure 6.5. Note, for example, the diagonal

$$9, 22, 35, 48, 61, 74,$$

which has common difference the Fibonacci number 13. Similarly, the diagonal

$$11, 19, 27, 35, 43, 51, 59$$

has common difference 8. Similar remarks hold for the florets of sunflowers, the scales of fir cones, and so on (see Adler [1977] and Fowler, Prusinkiewicz,and Battjes [1992]). Again, no explanation for why Fibonacci numbers arise in this aspect of phyllotaxis is known.

Example 6.8 "Hot Hand" (Example 2.32 Revisited) Recall the basketball phenomenon known as "hot hand." A hot hand assumes that once a player makes a shot, he or she has a higher-than-average chance of making the next shot. In Example 2.32 we considered the probability of all the made shots occurring consecutively. Here, we will consider the number of ways of making *no* consecutive shots.

If a player shoots n shots, there are 2^n possible outcomes; each shot can be either made or missed.[3] Let B_n denote the subset of those orderings of X's and O's that

[3] It does not follow that all 2^n orderings are equally likely. Made shots and missed shots are rarely equally likely.

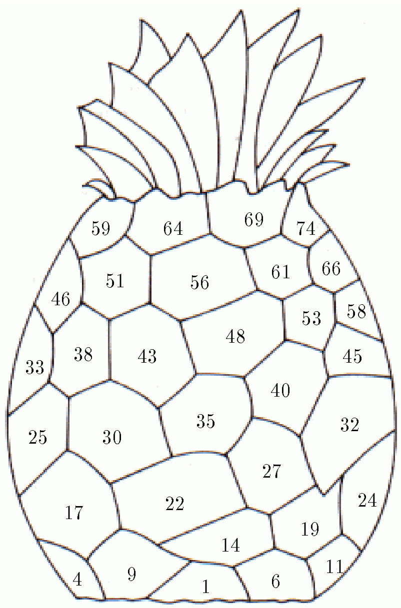

Figure 6.5: Fibonacci numbers and pineapples. (From Coxeter [1969]. Reprinted with permission of John Wiley & Sons, Inc.)

contain no consecutive made shots, i.e., no two consecutive X's. To find $b_n = |B_n|$, we refer to made shot i as c_i and let $C_n = \{c_1, c_2, \ldots, c_n\}$. Put another way, our question asks: How many subsets of C_n contain no c_i, c_{i+1}, $i = 1, 2, \ldots, n-1$? Let B be one such subset. Either B contains c_n or it does not. If it does, then $B - \{c_n\}$ is a subset of C_{n-2} since c_{n-1} is certainly not in B. If B does not contain c_n, then $B - \{c_n\} = B$ is a subset of C_{n-1}. Therefore, for $n \geq 2$,

$$b_n = b_{n-1} + b_{n-2}. \tag{6.12}$$

For $n = 1$, $b_1 = 2$; either the one shot is made or missed. If $n = 2$, then either no shot is made, the first shot is made and the second missed, or vice versa. Thus, $b_3 = 3$. Using these initial conditions, we see that the solution of recurrence (6.12) is closely related to the Fibonacci numbers. In particular,

$$b_n = F_{n+1}, \; n \geq 1. \qquad \blacksquare$$

Thus, if 10 shots are attempted (as in Example 2.32), only $b_{10} = F_{11} = 144$ out of $2^{10} = 1024$ outcomes contain no consecutive made shots.

6.1.3 Derangements

Example 6.9 The Hatcheck Problem Imagine that n gentlemen attend a party and check their hats. The checker has a little too much to drink, and returns the hats at random. What is the probability that no gentleman receives his own hat? How does this probability depend on the number of gentlemen? We shall answer these questions by studying the notion of a derangement. See Takács [1980] for the origin, the history, and alternative formulations of this problem. ■

Let n objects be labeled $1, 2, \ldots, n$. An arrangement or permutation in which object i is not placed in the ith place for any i is called a *derangement*. For example, if n is 3, then 231 is a derangement, but 213 is not since 3 is in the third place. Let D_n be the number of derangements of n objects.

Derangements arise in a card game (*rencontres*) where a deck of cards is laid out in a row on the table and a second deck is laid out randomly, one card on top of each of the cards of the first deck. The number of matching cards determines a score. In 1708, the Frenchman P. R. Montmort posed the problem of calculating the probability that no matches will take place and called it "le problème des rencontres," rencontre meaning "match" in French. This is, of course, the problem of calculating D_{52}. The problem of computing the number of matching cards will be taken up in Section 7.2. There we also discuss applications to the analysis of guessing abilities in psychic experiments. The first deck of cards corresponds to an unknown order of things selected or sampled, and the second to the order predicted by a psychic. In testing claims of psychic powers, one would like to compute the probability of getting matches right. The probability of getting at least one match right is 1 minus the probability of getting no matches right, that is, 1 minus the probability of getting a derangement.

Clearly, $D_1 = 0$: There is no arrangement of one element in which the element does not appear in its proper place. $D_2 = 1$: The only derangement is 21. We shall derive a recurrence relation for D_n. Suppose that there are $n+1$ elements, $1, 2, \ldots, n+1$. A derangement of these $n+1$ elements involves a choice of the first element and then an ordering of the remaining n. The first element can be any of n different elements: $2, 3, \ldots, n+1$. Suppose that k is put first. Then either 1 appears in the kth spot or it does not. If 1 appears in the kth spot, we have left the elements

$$2, 3, \ldots, k-1, k+1, \ldots, n+1,$$

and we wish to order them so that none appears in its proper location [see Figure 6.6(a)]. There are D_{n-1} ways to do this, since there are $n-1$ elements. Suppose next that 1 does not appear in the kth spot. We can think of first putting 1 into the kth spot [as shown in Figure 6.6(b)] and then deranging the elements in the second through $(n+1)$st spots. There are D_n such derangements. In sum, we have n choices for the element k which appears in the first spot. For each of these, we either choose an arrangement with 1 in the kth spot—which we can do in D_{n-1} ways—or we choose an arrangement with 1 not in the kth spot—which we can do in D_n ways. It follows by the product and sum rules that

$$D_{n+1} = n(D_{n-1} + D_n). \tag{6.13}$$

Equation (6.13) is a recurrence relation that makes sense for $n \geq 2$. If we add the

$$
\begin{array}{lccccccccc}
 & k & & & & 1 & & & & \\
(a) & \cdot & \cdots & & & \cdot & \cdots & & & \\
 & \text{1st} & & & & k\text{th} & & & & \\
\end{array}
$$

$$
\begin{array}{lcccccccccc}
 & k & 2 & 3 & & k-1 & 1 & k+1 & & n+1 \\
(b) & \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot & \cdots & \cdot \\
 & \text{1st} & \text{2nd} & \text{3rd} & & (k-1)\text{st} & k\text{th} & (k+1)\text{st} & & (n+1)\text{st} \\
\end{array}
$$

Figure 6.6: Derangements with k in the first spot and 1 in the kth spot and other elements (a) in arbitrary order and (b) in the proper spots.

initial conditions $D_1 = 0, D_2 = 1$, it turns out that

$$D_n = n!\left[1 - \frac{1}{1!} + \frac{1}{2!} - \frac{1}{3!} + \cdots + (-1)^n \frac{1}{n!}\right] \tag{6.14}$$

or (for $n \geq 2$),

$$D_n = n!\left[\frac{1}{2!} - \frac{1}{3!} + \cdots + (-1)^n \frac{1}{n!}\right]. \tag{6.15}$$

We shall see in Section 6.3.2 how to derive these formulas.

Let us now apply these formulas to the hatcheck problem of Example 6.9. Let p_n be the probability that no gentleman gets his hat back if there are n gentlemen. Then (for $n \geq 2$) we have

$$
\begin{aligned}
p_n &= \frac{\text{number of arrangements with no one receiving his own hat}}{\text{number of arrangements}} \\
&= \frac{D_n}{n!} \\
&= \left[\frac{1}{2!} - \frac{1}{3!} + \cdots + (-1)^n \frac{1}{n!}\right].
\end{aligned}
$$

Table 6.3 shows values of p_n for several n. Note that p_n seems to be converging rapidly. In fact, we can calculate exactly what p_n converges to. Recall that

$$e^x = 1 + x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \cdots$$

[see (5.3)]. Hence,

$$e^{-1} = \frac{1}{2!} - \frac{1}{3!} + \cdots,$$

so p_n converges to $e^{-1} = 0.367879441\ldots$. The convergence is so rapid that p_7 and p_8 already differ only in the fifth decimal place. The probability that no gentleman receives his hat back very rapidly becomes essentially independent of the number of gentlemen.

Table 6.3: Values of p_n

n	2	3	4	5	6	7	8
p_n	.500000	.333333	.375000	.366667	.368056	.367858	.367883

Example 6.10 Latin Rectangles In Chapter 1 we talked about Latin squares and their applications to experimental design, and in Exercise 15, Section 5.1, we introduced Latin rectangles and the idea of building up Latin squares one row at a time. Let $L(r, n)$ be the number of $r \times n$ Latin rectangles with entries $1, 2, \ldots, n$. (Recall that such a rectangle is an $r \times n$ array with entries $1, 2, \ldots, n$ so that no two entries in any row or column are the same.) Let $K(r, n)$ be the number of $r \times n$ Latin rectangles with entries $1, 2, \ldots, n$ and first row in the *standard position* $123 \cdots n$. Then

$$L(r, n) = n!K(r, n), \tag{6.16}$$

for one may obtain any Latin rectangle by finding one with a standard first row and then permuting the first row and performing the same permutation on the elements in all remaining rows.

We would like to calculate $L(r, n)$ or $K(r, n)$ for every r and n. By virtue of (6.16), these problems are equivalent. In Example 1.1, we asked for $L(5, 5)$ (which is 161,280; see Ryser [1963]). $K(2, n)$ is easy to calculate. It is simply D_n, the number of derangements of n elements. For we obtain the second row of a Latin rectangle with the first row in the standard position by deranging the elements of the first row.

Two formulas for $L(r, n)$ based on a function of certain matrices are given by Fu [1992]. (Shao and Wei [1992] gave an explicit formula for $L(n, n)$ based on an idea of MacMahon [1898].) ■

Example 6.11 DNA Sequence Alignment As noted in Section 2.17, mutations are a key process by which evolution takes place. Given DNA sequences from two different species, we sometimes try to see how close they are, and in particular look for patterns that appear in both. We often do this by aligning the two sequences, one under the other, so that a subsequence of each is (almost) the same. For instance, consider the sequences AATAATGAC and GAGTAATCGGAT. (Note that these have different lengths.) One alignment is the following:

$$\begin{array}{cccccccccccc} & A & A & T & A & A & T & G & A & C & & \\ G & A & G & T & A & A & T & C & G & G & A & T \end{array} \tag{6.17}$$

Here, we note a common subsequence TAAT. (In practical alignment applications, we often allow insertion and deletion of letters, but we will disregard that here.) Searching for good sequence alignments, ones where there are long common subsequences or patterns, has led to very important biological insights. For example, it was discovered that the sequence for platelet derived factor, which causes growth in the body, is 87 percent identical to the sequence for *v-sis*, a cancer-causing gene. This led to the discovery that *v-sis* works by stimulating growth. Indeed, as Gusfield [1997] points out, in DNA sequences (and, more generally, in other biomolecular sequences such as RNA or amino acid sequences), "high sequence similarity usually implies significant functional or structural similarity."

One way to measure how good an alignment of two sequences is is to count the number of positions where they don't match. This is called the *mismatch distance*. For instance, in alignment (6.17), the mismatch distance is 4 if we disregard places where the top sequence has no entries and 7 if we count places where one sequence has no entries. For more on sequence alignment in molecular biology, see Apostolico and Giancarlo [1999], Gusfield [1997], Myers [1995], Setubal and Meidanis [1997], or Waterman [1995].

Here we consider a simplified version of the sequence alignment problem. Suppose that we are given a DNA sequence of length n and it evolves by a random "permutation" of the elements into another such sequence. What is the probability that the mismatch distance between the two sequences is n? If the first sequence is AGCT, this is the probability that the new sequence is a derangement of the first, i.e., $D_4/4! = 3/8$. However, if the original sequence is AGCC, in which there are repeated entries, the problem is different. First, there are now only $4!/2! = 12$ possible sequences with these bases, not 4!. (Why?) Second, the only permutations of AGCC in which no element is in the same position as in AGCC are CCAG and CCGA. Thus, the desired probability is $\dfrac{2}{4!/2!} = \dfrac{1}{6}$, not $\dfrac{D_4}{4!} = \dfrac{3}{8}$. ■

6.1.4 Recurrences Involving More than One Sequence

Generalizing Example 6.4, let us define a codeword from the alphabet $\{0,1,2,3\}$ to be *legitimate* if and only if it has an even number of 0's *and* an even number of 3's. Let a_k be the number of legitimate codewords of length k. How do we find a_k? To answer this question, it turns out to be useful, in a manner analogous to the situation of Example 6.4, to consider other possibilities for a word of length k. Let b_k be the number of k-digit words from the alphabet $\{0,1,2,3\}$ with an even number of 0's and an odd number of 3's, c_k the number with an odd number of 0's and an even number of 3's, and d_k the number with an odd number of 0's and an odd number of 3's. Note that

$$d_k = 4^k - a_k - b_k - c_k. \tag{6.18}$$

Observe that we get a legitimate codeword of length $k+1$ by preceding a legitimate codeword of length k by a 1 or a 2, by preceding a word of length k with an even number of 0's and an odd number of 3's with a 3, or by preceding a word of length k with an odd number of 0's and an even number of 3's with a 0. Hence,

$$a_{k+1} = 2a_k + b_k + c_k. \tag{6.19}$$

Similarly,

$$b_{k+1} = a_k + 2b_k + d_k, \tag{6.20}$$

or, using (6.18),

$$b_{k+1} = b_k - c_k + 4^k. \tag{6.21}$$

Finally,

$$c_{k+1} = a_k + 2c_k + d_k, \tag{6.22}$$

or

$$c_{k+1} = c_k - b_k + 4^k. \tag{6.23}$$

Equations (6.19), (6.21), and (6.23) can be used together to compute any desired value a_k. We start with the initial conditions $a_1 = 2, b_1 = 1, c_1 = 1$. From (6.19), (6.21), (6.23), we compute

$$\begin{aligned} a_2 &= 2 \cdot 2 + 1 + 1 = 6, \\ b_2 &= 1 - 1 + 4^1 = 4, \\ c_2 &= 1 - 1 + 4^1 = 4. \end{aligned}$$

These results are easy to check by listing the corresponding sequences. For instance, the six sequences from $\{0, 1, 2, 3\}$ of length 2 and having an even number of 0's and 3's are $00, 33, 11, 12, 21, 22$. Similarly, one obtains

$$\begin{aligned} a_3 &= 2 \cdot 6 + 4 + 4 = 20, \\ b_3 &= 4 - 4 + 4^2 = 16, \\ c_3 &= 4 - 4 + 4^2 = 16. \end{aligned}$$

Notice that we have not found a single recurrence relation. However, we have found three relations that may be used simultaneously to compute the desired numbers.

EXERCISES FOR SECTION 6.1

1. Suppose that $a_n = 4a_{n-1} + 3, n \geq 1$, and $a_1 = 5$. Derive a_5 and a_6.
2. In Example 6.3 with $r = .2$, $S_0 = \$5000$, and simple interest, use the recurrence successively to compute S_1, S_2, S_3, S_4, S_5, and S_6, and check your answer by using the equation $S_k = S_0(1 + kr)$.
3. Repeat Exercise 2 for compound interest and use the equation $S_k = (1 + r)^k S_0$ to check your answer.
4. In Example 6.4:

   (a) Derive a_4. (b) Derive a_5.

   (c) Verify that $a_2 = 10$ by listing all legitimate codewords of length 2.

   (d) Repeat part (c) for $a_3 = 36$.
5. Check the formula in Example 6.6 for b_3 by explicitly listing all of the permutations of $\{1, 2, 3\}$ and the number of permutations needed to transform the identity permutation into each.
6. In Example 6.7, verify that $f(4) = 11$ by drawing four lines in the plane and labeling the regions.

7. Find a solution to the recurrence (6.5) under the initial condition $f(1) = 15$.
8. Find two different solutions to the recurrence (6.6).
9. In Example 6.8, calculate b_4 and b_5, and verify your answers by enumerating the ways to shoot 4 and 5 shots with none made consecutively.
10. Find a solution to the recurrence (6.13) different from the sequence defined by (6.14).
11. Find all derangements of $\{1, 2, 3, 4\}$.
12. In the example of Section 6.1.4, use the recurrences (6.19), (6.21), and (6.23) to compute a_4, b_4, and c_4.
13. On the first day, n jobs are to be assigned to n workers. On the second day, the jobs are again to be assigned, but no worker is to get the same job that he or she had on the first day. In how many ways can the jobs be assigned for the two days?
14. In a computer system overhaul, a bank employee mistakenly deleted records of seven "pin numbers" belonging to seven accounts. After recreating the records, he assigned those pins to the accounts at random. In how many ways could he do this so that:

    (a) At least one pin gets properly assigned?

    (b) All seven pins get properly assigned?

15. A lab director can run two different kinds of experiments, the expensive one (E) costing \$8000 and the inexpensive one (I) costing \$4000. If, for example, she has a budget of \$12,000, she can perform experiments in the following sequences: III, IE, or EI. Let $F(n)$ be the number of sequences of experiments she can run spending exactly \$$n$. Thus, $F(12{,}000) = 3$.

    (a) Find a recurrence for $F(n)$.

    (b) Suppose that there are p different kinds of experiments, $E_1, E_2, \ldots, E_p$, with E_i costing d_i dollars to run. Find a recurrence for $F(n)$ in this case.

16. Suppose that we have 10¢ stamps, 18¢ stamps, and 28¢ stamps, each in unlimited supply. Let $f(n)$ be the number of ways of obtaining n cents of postage if the order in which we put on stamps counts. For example, $f(10) = 1$ and $f(20) = 1$ (two 10¢ stamps), while $f(28) = 3$ (one 28¢ stamp, or a 10¢ stamp followed by an 18¢ stamp, or an 18¢ stamp followed by a 10¢ stamp).

    (a) If $n > 29$, derive a recurrence for $f(n)$.

    (b) *Use the recurrence* of part (a) to find the number of ways of obtaining 66¢ of postage.

    (c) Check your answer to part (b) by writing down all the ways.

17. An industrial plant has two sections. Suppose that in one week, nine workers are assigned to nine different jobs in the first section and another nine workers are assigned to nine different jobs in the second section. In the next week, the supervisor would like to reassign jobs so that no worker gets back his or her old job. (No two jobs in the plant are considered the same.)

    (a) In how many ways can this be done if each worker stays in the same section of the plant?

(b) In how many ways can this be done if each worker is shifted to a section of the plant different from the one in which he or she previously worked?

18. In predicting future sales of a product, one (probably incorrect) assumption is to say that the amount sold next year will be the average of the amount sold this year and last year. Suppose that a_n is the amount sold in year n.

    (a) Find a recurrence for a_n. (b) Solve the recurrence if $a_0 = a_1 = 1$.

19. Find the number of derangements of $\{1, 2, 3, 4, 5, 6, 7, 8\}$ in which the first four elements are mapped into:

    (a) 1, 2, 3, 4 in some order (b) 5, 6, 7, 8 in some order

20. Suppose that $f(p)$ is the number of comparisons required to sort p items using the algorithm bubble sort (Section 3.6.4). Find a recurrence for $f(p)$ and solve.

21. A codeword from the alphabet $\{0, 1, 2\}$ is considered legitimate if and only if no two 0's appear consecutively. Find a recurrence for the number b_n of legitimate codewords of length n.

22. A codeword from the alphabet $\{0, 1, 2\}$ is considered legitimate if and only if there is an even number of 0's and an odd number of 1's. Find simultaneous recurrences from which it is possible to compute the number of legitimate codewords of length n.

23. (a) How many permutations of the integers $1, 2, \ldots, 9$ put each even integer into its natural position and no odd integer into its natural position?

    (b) How many permutations of the integers $1, 2, \ldots, 9$ have exactly four numbers in their natural position?

24. In a singles tennis tournament, $2n$ players are paired off in n matches, and $f(n)$ is the number of different ways in which this pairing can be done. Determine a recurrence for $f(n)$.

25. Suppose that a random permutation of the following DNA sequences occurs. What is the probability that the mismatch distance between the original and permuted sequences is n?

    (a) AGT (b) AACC (c) ACTCGC
    (d) ACTGGGG (e) CTTAAA (f) CTAGG

26. Suppose that

$$a_n = \begin{cases} a_{n-1} & n \text{ even} \\ 2a_{n-2} + a_{n-4} + \cdots + a_3 + a_1 + 1 & n \text{ odd.} \end{cases}$$

    If $a_1 = 1$ and $a_3 = 3$, prove by induction that $a_{2n} = a_{2n-1} = F_{2n-1}$, i.e., $a_n =$ the Fibonacci number $F_{2\lfloor\frac{n+1}{2}\rfloor - 1}$.

27. (a) Suppose that chairs are arranged in a circle. Let L_n count the number of subsets of n chairs which don't contain consecutive chairs. Show that

$$L_{n+1} = F_n + F_{n+2}.$$

    (The numbers L_n are called *Lucas numbers*.[4])

[4]Édouard Lucas (1842–1891), was a French mathematician who attached Fibonacci's name to the sequence solution to Fibonacci's rabbit problem posed in *Liber Abaci*.

(b) Determine two initial conditions for L_n, namely, L_1 and L_2.

(c) Prove that $L_n = L_{n-1} + L_{n-2}$.

28. (a) Prove that the number of ways to write n as the sum of 1's and 2's is equal to the Fibonacci number F_n.

    (b) How many different ways can you put \$1.00 into a vending machine using only nickels and dimes?

29. In our notation, F_{n-1} is the nth Fibonacci number since we start with $F_0 = 1$.

    (a) Prove that every third Fibonacci number is divisible by $F_2 = 2$.

    (b) Prove that every fourth Fibonacci number is divisible by $F_3 = 3$.

    (c) Prove that every fifth Fibonacci number is divisible by $F_4 = 5$.

    (d) Prove that every nth Fibonacci number is divisible by F_{n-1}.

30. Consider the Fibonacci numbers F_n, $n = 0, 1, \ldots$.

    (a) Prove that $F_{n-1}F_n - F_{n-2}F_{n+1} = (-1)^n$.

    (b) Prove that $F_{n+1}F_{n-1} - F_n^2 = (-1)^n$.

    (c) Prove that $F_n = 2 + \displaystyle\sum_{k=1}^{n-2} F_k$.

    (d) Prove that $F_{2n+1} = 1 + \displaystyle\sum_{k=1}^{n} F_{2k}$.

    (e) Prove that $F_{n+1} = \displaystyle\sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n-k}{k}$.

    (f) Prove that $F_{n+m} = F_m F_{n+1} + F_{m-1}F_n$.

    (g) Prove that $F_{2n+1} = F_n^2 + F_{n+1}^2$.

31. If F_n is the nth Fibonacci number, find a simple, closed-form expression for

$$F_1 + F_2 + \cdots + F_n$$

which involves F_p for only one p.

32. Let $S(n,t)$ denote the number of ways to partition an n-element set into t nonempty, unordered subsets.[5] Then $S(n,t)$ satisfies

$$S(n,t) = tS(n-1,t) + S(n-1,t-1), \tag{6.24}$$

for $t = 1, 2, \ldots, n-1$. Equation (6.24) is an example of a recurrence involving two indices. We could use it to solve for any $S(n,t)$. For instance, suppose that we start with the observation that $S(n,1) = 1$, all n, and $S(n,n) = 1$, all n. Then we can compute $S(n,t)$ for all remaining n and $t \leq n$. For $S(3,2)$ can be computed from $S(2,2)$ and $S(2,1)$; $S(4,2)$ from $S(3,2)$ and $S(3,1)$; $S(4,3)$ from $S(3,3)$ and $S(3,2)$; and so on.

[5] $S(n,t)$ is called a Stirling number of the second kind and was discussed in Sections 2.10.4 and 5.5.3.

(a) Compute $S(5,3)$ by using (6.24). (b) Compute $S(6,3)$.

(c) Show that (6.24) holds.

33. In Exercise 24 of the Additional Exercises for Chapter 2, consider a grid with m north-south streets and n east-west streets. Let $s(m,n)$ be the number of different routes from point A to point B if A and B are located as in Figure 2.7. Find a recurrence for $s(m+1,n+1)$.

34. Determine a recurrence relation for $f(n)$, the number of regions into which the plane is divided by n circles each pair of which intersect in exactly two points and no three of which meet in a single point.

35. (a) Suppose that $f(n+1) = f(n)f(n-1)$, all $n \geq 1$, and $f(0) = f(1) = 2$. Find $f(n)$.

    (b) Repeat part (a) if $f(0) = f(1) = 1$.

36. In Example 6.6 we calculated b_n, the average number of transpositions needed to transform the identity permutation into a randomly chosen permutation of $\{1, 2, \ldots, n\}$. This was under the assumption that each permutation of $\{1, 2, \ldots, n\}$ is equally likely to be chosen. Calculate b_n if the identity permutation is twice as likely to be chosen over any other permutation and all other permutations are equally likely to be chosen.

37. (Liu [1968]) A *pattern* in a bit string consists of a number of consecutive digits, for example, 011. A pattern is said to *occur* at the kth digit of a bit string if when scanning the string from left to right, the full pattern appears after the kth digit has been scanned. Once a pattern occurs, that is, is observed, scanning begins again. For example, in the bit string 110101010101, the pattern 010 occurs at the fifth and ninth digits, but not at the seventh digit. Let b_n denote the number of n-digit bit strings with the pattern 010 occurring at the nth digit. Find a recurrence for b_n. (*Hint:* Consider the number of bit strings of length n ending in 010, and divide these into those where the 010 pattern occurs at the nth digit and those where it does not.)

38. Suppose that B is an $n \times n$ board and $r_n(B)$ is the coefficient of x^n in the rook polynomial $R(x,B)$. Use recurrence relations to compute $r_n(B)$ if

    (a) B has all squares darkened;

    (b) B has only the main diagonal lightened.

39. In the example of Section 6.1.4, find a single recurrence for a_k in terms of earlier values of a_p only.

40. Suppose that C_k is the number of connected, labeled graphs of k vertices. Harary and Palmer [1973] derive the recurrence

$$C_k = 2^{\binom{k}{2}} - \frac{1}{k}\sum_{p=1}^{k-1}\binom{k}{p}C_p p 2^{\binom{k-p}{2}}.$$

    Using the fact that $C_1 = 1$, compute C_2, C_3, and C_4, and check your answers by drawing the graphs.

41. A sequence of p 0's, q 1's, and r 2's is considered "good" if there are no consecutive digits in the sequence which are the same. Let $N(p,q,r)$ be the number of such "good" sequences.

(a) Calculate $N(p,q,0)$.

(b) How many distinct sequences of p 0's, q 1's, and r 2's are possible if no restrictions are imposed?

(c) Find a recurrence relation for $N(p,q,r)$.

6.2 THE METHOD OF CHARACTERISTIC ROOTS

6.2.1 The Case of Distinct Roots

So far we have derived a number of interesting recurrence relations. Several of these we were able to solve by iterating back to the original values or initial conditions. Indeed, we could do something similar even with some of the more difficult recurrences we have encountered. There are no general methods for solving all recurrences. However, there are methods that work for a very broad class of recurrences. In this section we investigate one such method, the method of characteristic roots. In Section 6.3 we show how to make use of the notion of generating function, developed in Chapter 5, for solving recurrences. The methods for solving recurrences were developed originally in the theory of difference equations. Careful treatments of difference equations can be found in Elaydi [1999], Goldberg [1958], or Kelley and Peterson [2001].

Consider the recurrence

$$a_n = c_1 a_{n-1} + c_2 a_{n-2} + \cdots + c_p a_{n-p}, \tag{6.25}$$

$n \geq p$, where $c_1, c_2, \ldots, c_p$ are constants and $c_p \neq 0$. Such a recurrence is called *linear* because all terms a_k occur to the first power and it is called *homogeneous*[6] because there is no term on the right-hand side that does not involve some a_k, $n-p \leq k \leq n-1$. Since the coefficients c_i are constants, the recurrence (6.25) is called a *linear homogeneous recurrence relation with constant coefficients.* The recurrences (6.1), (6.7), (6.9), and (6.11) are examples of such recurrences. The recurrences (6.4), (6.5), (6.6), (6.8), and (6.10) are not homogeneous and the recurrence (6.13) does not have constant coefficients. All of the recurrences we have encountered so far are linear.

We shall present a technique for solving linear homogeneous recurrence relations with constant coefficients; it is very similar to that used to solve linear differential equations with constant coefficients, as the reader who is familiar with the latter technique will see.

A recurrence (6.25) has a unique solution once we specify the values of the first p terms, $a_0, a_1, \ldots, a_{p-1}$; these values form the *initial conditions.* From a_0, a_1, $\ldots, a_{p-1}$, we can use the recurrence to find a_p. Then from $a_1, a_2, \ldots, a_p$, we can use the recurrence to find a_{p+1}, and so on.

In general, a recurrence (6.25) has many solutions, if the initial conditions are disregarded. Some of these solutions will be sequences of the form

$$\alpha^0, \alpha^1, \alpha^2, \ldots, \alpha^n, \ldots, \tag{6.26}$$

[6] We have previously defined homogeneous but in the context of polynomials.

where α is a number. We begin by finding values of α for which (6.26) is a solution to the recurrence (6.25). In (6.25), let us substitute x^k for a_k and solve for x. Making this substitution, we get the equation

$$x^n - c_1 x^{n-1} - c_2 x^{n-2} - \cdots - c_p x^{n-p} = 0. \tag{6.27}$$

Dividing both sides of (6.27) by x^{n-p}, we obtain

$$x^p - c_1 x^{p-1} - c_2 x^{p-2} - \cdots - c_p = 0. \tag{6.28}$$

Equation (6.28) is called the *characteristic equation* of the recurrence (6.25). It is a polynomial in x of power p, so has p roots $\alpha_1, \alpha_2, \ldots, \alpha_p$. Some of these may be repeated roots and some may be complex numbers. These roots are called the *characteristic roots* of the recurrence (6.25). For instance, consider the recurrence

$$a_n = 5a_{n-1} - 6a_{n-2}, \tag{6.29}$$

with initial conditions $a_0 = 1, a_1 = 1$. Then $p = 2, c_1 = 5, c_2 = -6$, and the characteristic equation is given by

$$x^2 - 5x + 6 = 0.$$

This has roots $x = 2$ and $x = 3$, so $\alpha_1 = 2$ and $\alpha_2 = 3$ are the characteristic roots.

If α is a characteristic root of the recurrence (6.25), and if we take $a_n = \alpha^n$, it follows that the sequence (a_n) satisfies the recurrence. Thus, corresponding to each characteristic root, we have a solution to the recurrence. In (6.29), $a_n = 2^n$ and $a_n = 3^n$ give solutions. However, neither satisfies both initial conditions $a_0 = 1, a_1 = 1$.

The next important observation to be made is that if the sequences (a'_n) and (a''_n) both satisfy the recurrence (6.25) and if λ_1 and λ_2 are constants, then the sequence (a'''_n), where $a'''_n = \lambda_1 a'_n + \lambda_2 a''_n$, also is a solution to (6.25). In other words, a weighted sum of solutions is a solution. To see this, note that

$$a'_n = c_1 a'_{n-1} + c_2 a'_{n-2} + \cdots + c_p a'_{n-p} \tag{6.30}$$

and

$$a''_n = c_1 a''_{n-1} + c_2 a''_{n-2} + \cdots + c_p a''_{n-p}. \tag{6.31}$$

Multiplying (6.30) by λ_1 and (6.31) by λ_2 and adding gives us

$$\begin{aligned}
a'''_n &= \lambda_1 a'_n + \lambda_2 a''_n \\
&= \lambda_1(c_1 a'_{n-1} + c_2 a'_{n-2} + \cdots + c_p a'_{n-p}) + \lambda_2(c_1 a''_{n-1} + c_2 a''_{n-2} + \cdots + c_p a''_{n-p}) \\
&= c_1(\lambda_1 a'_{n-1} + \lambda_2 a''_{n-1}) + c_2(\lambda_1 a'_{n-2} + \lambda_2 a''_{n-2}) + \cdots + c_p(\lambda_1 a'_{n-p} + \lambda_2 a''_{n-p}) \\
&= c_1 a'''_{n-1} + c_2 a'''_{n-2} + \cdots + c_p a'''_{n-p}.
\end{aligned}$$

Thus, a'''_n does satisfy (6.25). For example, if we define $a_n = 3 \cdot 2^n + 8 \cdot 3^n$, it follows that a_n satisfies (6.29).

In general, suppose that $\alpha_1, \alpha_2, \ldots, \alpha_p$ are the characteristic roots of recurrence (6.25). Then our reasoning shows that if $\lambda_1, \lambda_2, \ldots, \lambda_p$ are constants, and if

$$a_n = \lambda_1 \alpha_1^n + \lambda_2 \alpha_2^n + \cdots + \lambda_p \alpha_p^n,$$

then a_n satisfies (6.25). It turns out that every solution of (6.25) can be expressed in this form, *provided that the roots* $\alpha_1, \alpha_2, \ldots, \alpha_p$ are distinct. For a proof of this fact, see the end of this subsection.

Theorem 6.1 Suppose that a linear homogeneous recurrence (6.25) with constant coefficients has characteristic roots $\alpha_1, \alpha_2, \ldots, \alpha_p$. Then if $\lambda_1, \lambda_2, \ldots, \lambda_p$ are constants, every expression of the form

$$a_n = \lambda_1 \alpha_1^n + \lambda_2 \alpha_2^n + \cdots + \lambda_p \alpha_p^n \tag{6.32}$$

is a solution to the recurrence. Moreover, if the characteristic roots are distinct, every solution to the recurrence has the form (6.32) for some constants $\lambda_1, \lambda_2, \ldots, \lambda_p$.

We call the expression in (6.32) the *general solution* of the recurrence (6.25).

It follows from Theorem 6.1 that to find the unique solution of a recurrence (6.25) subject to initial conditions $a_0, a_1, \ldots, a_{p-1}$, if the characteristic roots are distinct, we simply need to find values for the constants $\lambda_1, \lambda_2, \ldots, \lambda_p$ in the general solution so that the initial conditions are satisfied. Let us see how to find these λ_i. In (6.29), every solution has the form

$$a_n = \lambda_1 2^n + \lambda_2 3^n.$$

Now we have

$$a_0 = \lambda_1 2^0 + \lambda_2 3^0, a_1 = \lambda_1 2^1 + \lambda_2 3^1.$$

So, from $a_0 = 1$ and $a_1 = 1$, we get the system of equations

$$\begin{aligned} \lambda_1 + \lambda_2 &= 1 \\ 2\lambda_1 + 3\lambda_2 &= 1. \end{aligned}$$

This system has the unique solution $\lambda_1 = 2, \lambda_2 = -1$. Hence, since $\alpha_1 \neq \alpha_2$, the unique solution to (6.29) with the given initial conditions is $a_n = 2 \cdot 2^n - 3^n$.

The general procedure works just as in this example. If we define a_n by (6.32), we use the initial values of $a_0, a_1, \ldots, a_{p-1}$ to set up a system of p simultaneous equations in the p unknowns $\lambda_1, \lambda_2, \ldots, \lambda_p$. One can show that *if* $\alpha_1, \alpha_2, \ldots, \alpha_p$ are distinct, this system always has a unique solution. The proof of this is the essence of the rest of the proof of Theorem 6.1, which we shall now present.

We close this subsection by sketching a proof of the statement in Theorem 6.1 that if the characteristic roots $\alpha_1, \alpha_2, \ldots, \alpha_p$ are distinct, every solution of a recurrence (6.25) has the form (6.32) for some constants $\lambda_1, \lambda_2, \ldots, \lambda_p$.[7] Suppose that

$$b_n = \lambda_1 \alpha_1^n + \lambda_2 \alpha_2^n + \cdots + \lambda_p \alpha_p^n$$

[7] The proof may be omitted.

is a solution to (6.25). Using the initial conditions $b_0 = a_0, b_1 = a_1, \ldots, b_{p-1} = a_{p-1}$, we find that

$$\left.\begin{array}{rcl} \lambda_1 + \lambda_2 + \cdots + \lambda_p &=& a_0 \\ \lambda_1\alpha_1 + \lambda_2\alpha_2 + \cdots + \lambda_p\alpha_p &=& a_1 \\ \lambda_1\alpha_1^2 + \lambda_2\alpha_2^2 + \cdots + \lambda_p\alpha_p^2 &=& a_2 \\ \vdots && \\ \lambda_1\alpha_1^{p-1} + \lambda_2\alpha_2^{p-1} + \cdots + \lambda_p\alpha_p^{p-1} &=& a_{p-1}. \end{array}\right\} \tag{6.33}$$

Equations (6.33) are a system of p linear equations in the p unknowns $\lambda_1, \lambda_2, \ldots, \lambda_p$. Consider now the matrix of coefficients of the system (6.33):

$$\begin{bmatrix} 1 & 1 & & 1 \\ \alpha_1 & \alpha_2 & & \alpha_p \\ \alpha_1^2 & \alpha_2^2 & \cdots & \alpha_p^2 \\ \vdots & \vdots & & \vdots \\ \alpha_1^{p-1} & \alpha_2^{p-1} & & \alpha_p^{p-1} \end{bmatrix}.$$

The determinant of this matrix is the famous *Vandermonde determinant.* One can show that the Vandermonde determinant is given by the product

$$\prod_{1 \le i < j \le p} (\alpha_j - \alpha_i),$$

the product of all terms $\alpha_j - \alpha_i$ with $1 \le i < j \le p$. Since $\alpha_1, \alpha_2, \ldots, \alpha_p$ are distinct, the determinant is not zero. Thus, there is a unique solution $\lambda_1, \lambda_2, \ldots, \lambda_p$ of the system (6.33). Hence, we see that a recurrence (6.25) with initial conditions $a_0, a_1, \ldots, a_{p-1}$ has a solution of the form (6.32). Now the recurrence with these initial conditions has just one solution, so this must be it. That completes the proof.

6.2.2 Computation of the *k*th Fibonacci Number

Let us illustrate the method with another example, the recurrence (6.11) for the Fibonacci numbers, which we repeat here:

$$F_k = F_{k-1} + F_{k-2}. \tag{6.34}$$

Here $p = 2$ and $c_1 = c_2 = 1$. The characteristic equation is given by $x^2 - x - 1 = 0$. By the quadratic formula, the roots of this equation, the characteristic roots, are given by $\alpha_1 = (1+\sqrt{5})/2$ and $\alpha_2 = (1-\sqrt{5})/2$. Because $\alpha_1 \neq \alpha_2$, the general solution is

$$\lambda_1 \left(\frac{1+\sqrt{5}}{2}\right)^k + \lambda_2 \left(\frac{1-\sqrt{5}}{2}\right)^k.$$

The initial conditions $F_0 = F_1 = 1$ give us the two equations

$$\lambda_1 + \lambda_2 = 1$$

and

$$\lambda_1\left(\frac{1+\sqrt{5}}{2}\right)+\lambda_2\left(\frac{1-\sqrt{5}}{2}\right)=1.$$

Solving these simultaneous equations for λ_1 and λ_2 gives us

$$\lambda_1=\frac{1}{\sqrt{5}}\left(\frac{1+\sqrt{5}}{2}\right),\quad \lambda_2=-\frac{1}{\sqrt{5}}\left(\frac{1-\sqrt{5}}{2}\right).$$

Hence, under the given initial conditions, the solution to (6.34), that is, the kth Fibonacci number, is given by

$$F_k=\frac{1}{\sqrt{5}}\left(\frac{1+\sqrt{5}}{2}\right)\left(\frac{1+\sqrt{5}}{2}\right)^k-\frac{1}{\sqrt{5}}\left(\frac{1-\sqrt{5}}{2}\right)\left(\frac{1-\sqrt{5}}{2}\right)^k,$$

or

$$F_k=\frac{\left(\frac{1+\sqrt{5}}{2}\right)^{k+1}-\left(\frac{1-\sqrt{5}}{2}\right)^{k+1}}{\sqrt{5}}, \tag{6.35}$$

or

$$F_k=\frac{\tau^{k+1}-(1-\tau)^{k+1}}{\sqrt{5}},$$

where τ is the golden ratio of Section 6.1.2. In Exercise 8 of Section 6.3, this result is derived using generating functions.

Example 6.12 Duration of Messages (Example 6.5 Revisited) We note next that the recurrences (6.9) and (6.34) are the same. Moreover, the initial conditions are the same. For $F_1=1$ and $F_2=2$, while $N_1=1$ and $N_2=2$. Also, for the same reason that we took F_0 to be 0, namely, to maintain the recurrence even for $k=2$, we take N_0 to be 0. Now as we observed earlier, if we are given a recurrence (6.25) that has distinct characteristic roots and initial conditions $a_0, a_1, \ldots, a_{p-1}$, the solution is determined uniquely. Hence, it follows that N_t must equal F_t for all $t \geq 0$, so we may use (6.35) to compute N_k. It is not too hard to show from this result that the Shannon capacity defined in Example 6.5 is given by

$$C=\log_2\left(\frac{1+\sqrt{5}}{2}\right).$$

■

6.2.3 The Case of Multiple Roots

Consider the recurrence

$$a_n=6a_{n-1}-9a_{n-2}, \tag{6.36}$$

with $a_0=1, a_1=2$. Its characteristic equation is $x^2-6x+9=0$, or $(x-3)^2=0$. The two characteristic roots are 3 and 3, that is, 3 is a multiple root. Hence, the second part of Theorem 6.1 does not apply. Whereas it is still true that 3^n is a solution of (6.36), and it is also true that $\lambda_1 3^n + \lambda_2 3^n$ is always a solution, it is not true that every solution of (6.36) takes the form $\lambda_1 3^n + \lambda_2 3^n$. In particular, there is no such solution satisfying our given initial conditions. For these conditions give us the equations

$$\begin{aligned} \lambda_1 + \lambda_2 &= 1 \\ 3\lambda_1 + 3\lambda_2 &= 2. \end{aligned}$$

There are no λ_1, λ_2 satisfying these two equations.

Suppose that α is a characteristic root of multiplicity u; that is, it appears as a root of the characteristic equation exactly u times. Then it turns out that not only does $a_n = \alpha^n$ satisfy the recurrence (6.25), but so do $a_n = n\alpha^n, a_n = n^2\alpha^n, \ldots,$ and $a_n = n^{u-1}\alpha^n$ (see Exercises 29, 30). In our example, 3 is a characteristic root of multiplicity $u = 2$, and both $a_n = 3^n$ and $a_n = n3^n$ are solutions of (6.25). Moreover, since a weighted sum of solutions is a solution and since both $a_n' = 3^n$ and $a_n'' = n3^n$ are solutions, so is $a_n''' = \lambda_1 3^n + \lambda_2 n 3^n$. Using this expression a_n''' and the initial conditions $a_0 = 1, a_1 = 2$, we get the equations

$$\begin{aligned} \lambda_1 &= 1 \\ 3\lambda_1 + 3\lambda_2 &= 2. \end{aligned}$$

These have the unique solution $\lambda_1 = 1, \lambda_2 = -\frac{1}{3}$. Hence, $a_n = 3^n - \frac{1}{3} \cdot n \cdot 3^n$ is a solution to the recurrence (6.36) with the initial conditions $a_0 = 1, a_1 = 2$. It follows that this must be the unique solution.

This procedure generalizes as follows. Suppose that a recurrence (6.25) has characteristic roots $\alpha_1, \alpha_2, \ldots, \alpha_q$, with α_i having multiplicity u_i. Then

$$\begin{gathered} \alpha_1^n, n\alpha_1^n, n^2\alpha_1^n, \ldots, n^{u_1-1}\alpha_1^n, \alpha_2^n, n\alpha_2^n, n^2\alpha_2^n, \ldots, n^{u_2-1}\alpha_2^n, \ldots, \\ \alpha_q^n, n\alpha_q^n, n^2\alpha_q^n, \ldots, n^{u_q-1}\alpha_q^n \end{gathered}$$

must all be solutions of the recurrence. Let us call these the *basic solutions*. There are p of these basic solutions in all. Let us denote them $b_1, b_2, \ldots, b_p$. Since a weighted sum of solutions is a solution, for any constants $\lambda_1, \lambda_2, \ldots, \lambda_p$,

$$a_n = \lambda_1 b_1 + \lambda_2 b_2 + \cdots + \lambda_p b_p$$

is also a solution of the recurrence. By a method analogous to that used to prove Theorem 6.1, one can show that every solution has this form for some constants $\lambda_1, \lambda_2, \ldots, \lambda_p$.

Theorem 6.2 Suppose that a linear homogeneous recurrence (6.25) with constant coefficients has basic solutions $b_1, b_2, \ldots, b_p$. Then the general solution is given by

$$a_n = \lambda_1 b_1 + \lambda_2 b_2 + \cdots + \lambda_p b_p, \tag{6.37}$$

for some constants $\lambda_1, \lambda_2, \ldots, \lambda_p$.

The unique solution satisfying initial conditions $a_0, a_1, \ldots, a_{p-1}$ can be computed by setting $n = 0, 1, \ldots, p-1$ in (6.37) and getting p simultaneous equations in the p unknowns $\lambda_1, \lambda_2, \ldots, \lambda_p$.

To illustrate, consider the recurrence

$$a_n = 7a_{n-1} - 16a_{n-2} + 12a_{n-3}, \tag{6.38}$$

$a_0 = 1, a_1 = 2, a_2 = 0$. Then the characteristic equation is

$$x^3 - 7x^2 + 16x - 12 = 0,$$

which factors as $(x-2)(x-2)(x-3) = 0$. The characteristic roots are therefore $\alpha_1 = 2$, with multiplicity $u_1 = 2$, and $\alpha_2 = 3$, with multiplicity $u_2 = 1$. Thus, the general solution to (6.38) has the form

$$a_n = \lambda_1\alpha_1^n + \lambda_2 n\alpha_1^n + \lambda_3\alpha_2^n = \lambda_1 2^n + \lambda_2 n2^n + \lambda_3 3^n.$$

Setting $n = 0, 1, 2$, we get

$$\begin{aligned} a_0 &= \lambda_1 + \lambda_3 = 1 \\ a_1 &= 2\lambda_1 + 2\lambda_2 + 3\lambda_3 = 2 \\ a_2 &= 4\lambda_1 + 8\lambda_2 + 9\lambda_3 = 0. \end{aligned}$$

This system has the unique solution $\lambda_1 = 5, \lambda_2 = 2, \lambda_3 = -4$. Hence, the unique solution to (6.38) with the given initial conditions is

$$a_n = 5 \cdot 2^n + 2 \cdot n2^n - 4 \cdot 3^n.$$

EXERCISES FOR SECTION 6.2

1. Which of the following recurrences are linear?

   (a) $a_n = 5a_{n-1} + 2a_{n-2} + 3$ (b) $b_n = 3b_{n-1} + 9b_{n-2} + 18b_{n-3} + 32b_{n-4}$
   (c) $c_n = 21c_{n-2} + 4c_{n-5}$ (d) $d_n = 16d_{n-1} - 12d_{n-2}$
   (e) $e_n = 24e_{n-1} + 22e_{n-2}^2$ (f) $f_n = nf_{n-1} + f_{n-2}$
   (g) $g_n = n^2 g_{n-2}$ (h) $h_n = 8h_{n-3} + 81$
   (i) $i_n = 5i_{n-1} + 3^n i_{n-2}$

2. Which of the recurrences in Exercise 1 are homogeneous?

3. Which of the recurrences in Exercise 1 have constant coefficients?

4. Use (6.35) to derive the values of F_k for $k = 2, 3, 4, 5, 6, 7$.

5. Find the characteristic equation of each of the following recurrences.

   (a) $a_n = -2a_{n-1} - a_{n-2}$ (b) $b_k = -7b_{k-1} + 18b_{k-2}$
   (c) $c_n = 3c_{n-1} + 18c_{n-2} - 7c_{n-3}$ (d) $d_n = 81d_{n-4} + 4d_{n-5}$
   (e) $e_k = 4e_{k-2}$ (f) $f_{n+1} = 2f_n + 3f_{n-1}$
   (g) $g_n = 18g_{n-7}$ (h) $h_n = 9h_{n-2}$
   (i) $i_n = i_{n-1} + 4i_{n-2} - 4i_{n-3}$ (j) $j_n = 2j_{n-1} + 9j_{n-2} - 18j_{n-3}$
   (k) $k_n = 11k_{n-1} + 22k_{n-2} + 11k_{n-3} - 33k_{n-8}$

6. In Exercise 5, find the characteristic roots of the recurrences of parts (a), (b), (e), (f), (h), (i), and (j). [*Hint:* 2 is a root in parts (i) and (j).]

7. (a) Show that the recurrence $a_n = 5a_{n-1}$ can have many solutions.
   (b) Show that this recurrence has a unique solution if we know that $a_0 = 20$.

8. Solve the following recurrences using the method of characteristic roots.

   (a) $a_n = 6a_{n-1}, a_0 = 5$ (b) $t_{k+1} = 2t_k, t_1 = 1$ (this is Example 6.1)

9. Consider the recurrence $a_n = 15a_{n-1} - 44a_{n-2}$. Show that each of the following sequences is a solution.

   (a) (4^n) (b) $(3 \cdot 11^n)$ (c) $(4^n - 11^n)$ (d) (4^{n+1})

10. In Exercise 9, which of the following sequences is a solution?
    (a) (-4^n) (b) $(4^n + 1)$ (c) $(3 \cdot 4^n + 12 \cdot 11^n)$
    (d) $(n4^n)$ (e) $(4^n 11^n)$ (f) $((-4)^n)$

11. Consider the recurrence $b_k = 7b_{k-1} - 10b_{k-2}$. Which of the following sequences is a solution?
    (a) (2^k) (b) $(5^k - 2^k)$ (c) $(2^k + 7)$
    (d) $(2^k - 5^k)$ (e) $(2^k + 5^{k+1})$

12. Use the method of characteristic roots to solve the following recurrences in Exercise 5 under the following initial conditions.

    (a) That of part (a) if $a_0 = 2, a_1 = 2$
    (b) That of part (b) if $b_0 = 0, b_1 = 8$
    (c) That of part (e) if $e_0 = -1, e_1 = 1$
    (d) That of part (f) if $f_0 = f_1 = 2$
    (e) That of part (h) if $h_0 = 4, h_1 = 2$
    (f) That of part (i) if $i_0 = 0, i_1 = 1, i_2 = 2$
    (g) That of part (j) if $j_0 = 2, j_1 = 1, j_2 = 0$

13. Suppose that in Example 6.5, a requires 2 units of time to transmit and b requires 3 units of time. Solve for N_t.

14. Solve for a_n in the product sales problem of Exercise 18, Section 6.1 if $a_0 = 0, a_1 = 1$.

15. Using (6.35), verify the results in Exercise 29, Section 6.1.

16. Using (6.35), verify the results in Exercise 30, Section 6.1.

17. Consider the recurrence $a_n = -a_{n-2}$.

    (a) Show that i and $-i$ are the characteristic roots. (*Note*: $i = \sqrt{-1}$.)
    (b) Is the sequence (i^n) a solution?
    (c) What about the sequence $(2i^n + (-i)^n)$?
    (d) Find the unique solution if $a_0 = 0, a_1 = 1$.

18. Consider the recurrence $a_n = -9a_{n-2}$.

(a) Find a general solution.

(b) Find the unique solution if $a_0 = 0, a_1 = 5$.

19. Consider the recurrence $F_n = 4F_{n-1} - 4F_{n-2}$. Show that there is a multiple characteristic root α and that for the initial conditions $F_0 = 1, F_1 = 3$, there are no constants λ_1 and λ_2 so that $F_n = \lambda_1\alpha^n + \lambda_2\alpha^n$ for all n.

20. Suppose that (a_n') and (a_n'') are two solutions of a recurrence (6.25) and that $a_n''' = a_n' - a_n''$. Is (a_n''') necessarily a solution to (6.25)? Why?

21. Suppose that (a_n'), (a_n''), and (a_n''') are three solutions to a recurrence (6.25) and that we have $b_n = \lambda_1 a_n' + \lambda_2 a_n'' + \lambda_3 a_n'''$. Is (b_n) necessarily a solution to (6.25)? Why?

22. Consider the recurrence

$$a_n = 9a_{n-1} - 27a_{n-2} + 27a_{n-3}.$$

Show that each of the following sequences is a solution.

(a) (3^n) (b) $(n3^n)$ (c) $(n^2 3^n)$
(d) $(3 \cdot 3^n)$ (e) $(3^n + n3^n)$ (f) $(4 \cdot 3^n + 8 \cdot n3^n - n^2 3^n)$

23. Consider the recurrence

$$a_n = 3a_{n-1} - 3a_{n-2} + a_{n-3}.$$

Show that each of the following sequences is a solution:

(a) $(1, 1, 1, \ldots)$ (b) $(0, 1, 2, 3, \ldots)$ (c) $(0, 1, 4, 9, \ldots)$

24. Consider the recurrence

$$b_n = 9b_{n-1} - 24b_{n-2} + 20b_{n-3}.$$

Show that each of the sequences (2^n), $(n2^n)$, and (5^n) is a solution.

25. Consider the recurrence

$$c_k = 13c_{k-1} - 60c_{k-2} + 112c_{k-3} - 64c_{k-4}.$$

Show that each of the following sequences is a solution.

(a) $(2, 2, \ldots)$ (b) $(3 \cdot 4^k)$ (c) $(4^k + k4^k + k^2 4^k)$
(d) $(4^k + 1)$ (e) $(k4^k - 11)$

26. Find the unique solution to:

(a) The recurrence of Exercise 22 if $a_0 = 0, a_1 = 1, a_2 = 1$

(b) The recurrence of Exercise 23 if $a_0 = 1, a_1 = 1, a_2 = 2$

(c) The recurrence of Exercise 24 if $b_0 = 1, b_1 = 2, b_2 = 0$

(d) The recurrence of Exercise 25 if $c_0 = c_1 = 0, c_2 = 10, c_3 = 0$

27. Solve the following recurrence relations under the given initial conditions.

(a) $a_n = 10a_{n-1} - 25a_{n-2}, a_0 = 1, a_1 = 2$

(b) $b_k = 14b_{k-1} - 49b_{k-2}, b_0 = 0, b_1 = 10$

(c) $c_n = 9c_{n-1} - 15c_{n-2} + 7c_{n-3}, c_0 = 0, c_1 = 1, c_2 = 2$ (*Hint:* $x = 1$ is a characteristic root.)

(d) $d_n = 13d_{n-1} - 40d_{n-2} + 36d_{n-3}, d_0 = d_1 = 1, d_2 = 0$ (*Hint:* $x = 2$ is a characteristic root.)

(e) $e_k = 10e_{k-1} - 37e_{k-2} + 60e_{k-3} - 36e_{k-4}, e_0 = e_1 = e_2 = 0, e_3 = 5$ (*Hint:* $x = 2$ and $x = 3$ are characteristic roots.)

28. Solve the following recurrence under the given initial condition.

$$a_n = -2a_{n-2} - a_{n-4}, \quad a_0 = 0, \quad a_1 = 1, \quad a_2 = 2, \quad a_3 = 3.$$

(*Hint:* $x = i$ and $x = -i$ are characteristic roots.)

29. Suppose that α is a characteristic root of the recurrence (6.25) and α has multiplicity 2. Show that (α^n) and $(n\alpha^n)$ are solutions to (6.25). [*Hint:* If $C(x) = 0$ is the characteristic equation, then $C(x) = (x - \alpha)^2 D(x)$ for some polynomial $D(x)$. If $C_n(x) = x^{n-p}C(x)$, show that α is a root of the derivative $C_n'(x)$. Substituting α for x in the equation $xC_n'(x) = 0$ shows that $(n\alpha^n)$ is a solution to (6.25).]

30. (a) Suppose that α is a characteristic root of the recurrence (6.25) and α has multiplicity 3. Show that $(\alpha^n), (n\alpha^n)$, and $(n^2\alpha^n)$ are solutions to (6.25). [*Hint:* Generalize the argument in Exercise 29 by noting that $C(x) = (x - \alpha)^3 D(x)$. Consider $C_n(x) = x^{n-p}C(x), A_n(x) = xC_n'(x)$, and $B_n(x) = xA_n'(x)$. Show that $(n\alpha^n)$ is a solution by considering $A_n(x) = 0$, and $(n^2\alpha^n)$ is a solution by considering $B_n(x) = 0$.]

(b) Generalize to the case where α is a characteristic root of multiplicity u.

6.3 SOLVING RECURRENCES USING GENERATING FUNCTIONS

6.3.1 The Method

Another method for solving recurrences uses the notion of generating function developed in Chapter 5. Suppose that $G(x)$ is the ordinary generating function for the sequence (a_k), that is, the function

$$G(x) = \sum_{k=0}^{\infty} a_k x^k.$$

We shall try to find (a_k) by finding its generating function. In particular, if we have a recurrence for a_k, the trick will be to multiply both sides of the recurrence by x^k and then take the sum, giving us an expression that can be used to derive $G(x)$.

Example 6.13 The Grains of Wheat (Example 6.1 Revisited) Let us illustrate the method with the recurrence relation of Example 6.1,

$$t_{k+1} = 2t_k. \tag{6.39}$$

The initial condition was $t_1 = 1$. In this case, t_0 is not defined. However, it will usually be convenient to think of our sequences as beginning with the zeroth term. Hence, we will try to define the early terms from the recurrence if they are not known or given. In particular, by (6.39), it is consistent to take

$$t_0 = \frac{1}{2}t_1 = \frac{1}{2}.$$

The ordinary generating function for (t_k) is

$$G(x) = \sum_{k=0}^{\infty} t_k x^k.$$

To derive $G(x)$, we start by multiplying both sides of the recurrence (6.39) by x_k, obtaining

$$t_{k+1}x^k = 2t_k x^k.$$

Then, we take sums:[8]

$$\sum_{k=0}^{\infty} t_{k+1}x^k = 2\sum_{k=0}^{\infty} t_k x^k. \tag{6.40}$$

The right-hand side of (6.40) is $2G(x)$. What is the left-hand side? We shall try to reduce that to an expression involving $G(x)$. Note that

$$\begin{aligned}
\textstyle\sum_{k=0}^{\infty} t_{k+1}x^k &= t_1 + t_2x + t_3x^2 + \cdots \\
&= \frac{1}{x}\left[t_1x + t_2x^2 + t_3x^3 + \cdots\right] \\
&= \frac{1}{x}\left[t_0 + t_1x + t_2x^2 + t_3x^3 + \cdots\right] - \frac{1}{x}t_0 \\
&= \frac{1}{x}\left[G(x) - t_0\right].
\end{aligned}$$

Hence,

$$\sum_{k=0}^{\infty} t_{k+1}x_k = \frac{G(x) - t_0}{x}. \tag{6.41}$$

Equations (6.40) and (6.41) now give us the equation

$$\frac{G(x) - t_0}{x} = 2G(x).$$

This equation, a *functional equation* for $G(x)$, can be solved for $G(x)$. A little bit of algebraic manipulation gives us

$$G(x) = \frac{t_0}{1-2x}.$$

[8] The sums may be taken over all values of k for which the recurrence applies. In some cases, it will be better or more appropriate to take the sum from $k = 1$ or from $k = 2$, and so on.

Since we have computed $t_0 = \frac{1}{2}$, we have

$$G(x) = \frac{1}{2}(1 - 2x)^{-1}.$$

Knowing $G(x)$, we can compute the desired value of t_k from it. The number t_k is given by the coefficient of x^k if we expand out $G(x)$. How can we expand $G(x)$? There are two methods. The easiest is to use the identity

$$1 + y + y^2 + \cdots + y^n + \cdots = \frac{1}{1-y}, \tag{6.42}$$

$|y| < 1$ [see Equation (5.2)]. Doing so gives us the result

$$G(x) = \frac{1}{2}\left[1 + (2x) + (2x)^2 + \cdots + (2x)^n + \cdots\right]$$

or

$$G(x) = \frac{1}{2} + x + 2x^2 + \cdots + 2^{n-1}x^n + \cdots.$$

In other words,

$$t_k = 2^{k-1},$$

which agrees with our earlier computation. An alternative way of expanding $G(x)$ is to use the Binomial Theorem (Theorem 5.3). We leave it to the reader to try this. ■

Example 6.14 Legitimate Codewords (Example 6.4 Revisited) Let us now illustrate the method with the following recurrence of Example 6.4:

$$a_{k+1} = 2a_k + 4^k. \tag{6.43}$$

We use the ordinary generating function

$$G(x) = \sum_{k=0}^{\infty} a_k x^k.$$

We know that $a_1 = 3$. From the recurrence, we can derive a_0 even though a_0 is not defined. We obtain

$$\begin{aligned} a_1 &= 2a_0 + 4^0, \\ 3 &= 2a_0 + 1, \\ a_0 &= 1. \end{aligned}$$

We now multiply both sides of the recurrence (6.43) by x^k and sum, obtaining

$$\sum_{k=0}^{\infty} a_{k+1}x^k = 2\sum_{k=0}^{\infty} a_k x^k + \sum_{k=0}^{\infty} 4^k x^k. \tag{6.44}$$

The left-hand side of (6.44) is given by

$$\frac{1}{x}\sum_{k=0}^{\infty} a_{k+1}x^{k+1} = \frac{1}{x}\left[G(x) - a_0\right] = \frac{1}{x}\left[G(x) - 1\right].$$

Hence, we obtain

$$\frac{1}{x}\left[G(x) - 1\right] = 2G(x) + \sum_{k=0}^{\infty}(4x)^k. \tag{6.45}$$

From the identity (6.42), we can rewrite this as

$$\frac{1}{x}\left[G(x) - 1\right] = 2G(x) + \frac{1}{1-4x}.$$

From this functional equation, it is simply a matter of algebraic manipulation to solve for $G(x)$. We obtain

$$\begin{aligned} G(x) - 1 &= 2xG(x) + \frac{x}{1-4x}, \\ G(x)(1-2x) &= 1 + \frac{x}{1-4x}, \\ G(x) &= \frac{1}{1-2x}\left(1 + \frac{x}{1-4x}\right), \\ G(x) &= \frac{1}{1-2x} + \frac{x}{(1-2x)(1-4x)}. \end{aligned} \tag{6.46}$$

This gives us the generating function for (a_k). How do we find a_k? It is easy enough to expand out the first term on the right-hand side of (6.46). The second term we expand by the method of partial fractions.[9] Namely, the second term on the right-hand side can be expressed as

$$\frac{a}{1-2x} + \frac{b}{1-4x}$$

for appropriate a and b. We compute that

$$a = -\frac{1}{2}, \quad b = \frac{1}{2}.$$

Thus,

$$G(x) = \frac{1}{1-2x} + \frac{-\frac{1}{2}}{1-2x} + \frac{\frac{1}{2}}{1-4x} = \frac{\frac{1}{2}}{1-2x} + \frac{\frac{1}{2}}{1-4x}. \tag{6.47}$$

To expand (6.47), we again use the identity (6.42), obtaining

$$G(x) = \frac{1}{2}\sum_{k=0}^{\infty}(2x)^k + \frac{1}{2}\sum_{k=0}^{\infty}(4x)^k.$$

[9] See most calculus texts for a discussion of this method.

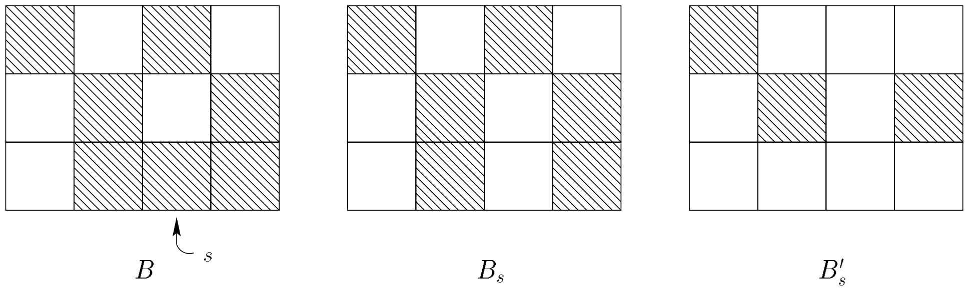

Figure 6.7: A board B, a square s [the $(3,3)$ square], and the boards B_s and B'_s obtained from board B and square s.

Thus, the coefficient of x^k is given by

$$a_k = \frac{1}{2}(2)^k + \frac{1}{2}(4)^k.$$

In particular, we can check our computation in Section 6.1. We have

$$\begin{aligned} a_2 &= \tfrac{1}{2}(2)^2 + \tfrac{1}{2}(4)^2 = 10, \\ a_3 &= \tfrac{1}{2}(2)^3 + \tfrac{1}{2}(4)^3 = 36. \end{aligned}$$

The reader might wish to check our results in still another way, namely by computing an exponential generating function for a_k directly by the methods of Section 5.5. ■

Example 6.15 Rook Polynomials[10] In Examples 5.10 and 5.14, we introduced rook polynomials and stated a result that would reduce computation of a rook polynomial of a board B to computation of the rook polynomials of "simpler" boards. Here we state another such result. Suppose that s is any darkened square of the board B. Let B_s be obtained from B by forbidding s (lightening s) and let B'_s be obtained from B by forbidding all squares in the same row or column as s. Figure 6.7 shows a board B, a square s, and the boards B_s and B'_s.

Note that to place $k \geq 1$ rooks on B, we either use square s or we do not. If we do not use square s, we have to place k rooks on the squares of B_s. If we use square s, we have $k-1$ rooks still to place, and we may use any darkened square of B except those in the same row or column as s; that is, we may use any darkened square of B'_s. Thus, by the sum rule of Chapter 2,

$$r_k(B) = r_k(B_s) + r_{k-1}(B'_s) \tag{6.48}$$

for $k \geq 1$. If we multiply both sides of (6.48) by x^k and sum over all $k \geq 1$, we find that

$$\sum_{k=1}^{\infty} r_k(B)x^k = \sum_{k=1}^{\infty} r_k(B_s)x^k + \sum_{k=1}^{\infty} r_{k-1}(B'_s)x^k. \tag{6.49}$$

[10] This example may be omitted if the reader has skipped Chapter 5.

The term on the left-hand side of (6.49) is just

$$R(x, B) - r_0(B) = R(x, B) - 1,$$

since $r_0(B) = 1$ for all boards B. The first term on the right-hand side is

$$R(x, B_s) - r_0(B_s) = R(x, B_s) - 1.$$

The second term on the right-hand side is equal to

$$x \sum_{k=1}^{\infty} r_{k-1}(B_s')x^{k-1} = x \sum_{k=0}^{\infty} r_k(B_s')x^k = xR(x, B_s').$$

Thus, (6.49) gives us

$$R(x, B) - 1 = R(x, B_s) - 1 + xR(x, B_s'),$$

or

$$R(x, B) = R(x, B_s) + xR(x, B_s'). \tag{6.50}$$

Application of this result to the board B of Figure 6.7 is left as an exercise (Exercise 27). ■

The method used in the preceding three examples can be applied to solve a variety of recurrences. It will always work on any recurrence like (6.25) which is linear and homogeneous with constant coefficients.[11] The result will give a generating function $G(x)$ of the form

$$\frac{p(x)}{q(x)},$$

where $p(x)$ is a polynomial of degree less than p and $q(x)$ is a polynomial of degree p and constant term equal to 1. [The polynomials $p(x)$ and $q(x)$ can be expressed in terms of the coefficients $c_1, c_2, \ldots, c_p$ and initial conditions $a_0, a_1, \ldots, a_{p-1}$ of the recurrence (6.25). See Brualdi [1999] or Exercise 25 for details.] If all the roots of $q(x)$ are real numbers, one can then use the method of partial fractions to express $p(x)/q(x)$ as a sum of terms of the form

$$\frac{\alpha}{(1 - \beta x)^t},$$

where t is a positive integer and α and β are real numbers. In turn, the terms

$$\frac{\alpha}{(1 - \beta x)^t}$$

can be expanded out using the Binomial Theorem, giving us

$$\frac{\alpha}{(1 - \beta x)^t} = \alpha \sum_{k=0}^{\infty} \binom{t + k - 1}{k} \beta^k x^k. \tag{6.51}$$

[11] The rest of this subsection may be omitted on first reading.

This also follows directly by using βx in place of x in Corollary 5.4.1.

If $q(x)$ has complex roots, the method of partial fractions can be used to express $p(x)/q(x)$ as a sum of terms of the form

$$\frac{a}{(x-b)^t} \quad \text{or} \quad \frac{ax+b}{(x^2+cx+d)^t},$$

where t is a positive integer and a, b, c, and d are real numbers. The former terms can be changed into terms of the form

$$\frac{\alpha}{(1-\beta x)^t}.$$

The latter terms can be manipulated by completing the square in the denominator and then using the expansion for

$$\frac{1}{(1+y^2)^t} = \frac{1}{[1-(-y^2)]^t}.$$

We omit the details.

6.3.2 Derangements

Let us next use the techniques of this section to derive the formula for the number of derangements D_n of n elements. We have the recurrence

$$D_{n+1} = n(D_{n-1} + D_n), \tag{6.52}$$

$n \geq 2$. We know that $D_2 = 1$ and $D_1 = 0$. Hence, using the recurrence (6.52), we derive $D_0 = 1$. With $D_0 = 1$, (6.52) holds for $n \geq 1$. The recurrence (6.52) is inconvenient because it expresses D_{n+1} in terms of both D_n and D_{n-1}. Some algebraic manipulation reduces (6.52) to the recurrence

$$D_{n+1} = (n+1)D_n + (-1)^{n+1}, \tag{6.53}$$

$n \geq 0$. For a detailed verification of this fact, see the end of this subsection.

Let us try to calculate the ordinary generating function

$$G(x) = \sum_{n=0}^{\infty} D_n x^n.$$

We multiply (6.53) by x^n and sum, obtaining

$$\sum_{n=0}^{\infty} D_{n+1} x^n = \sum_{n=0}^{\infty} (n+1) D_n x^n + \sum_{n=0}^{\infty} (-1)^{n+1} x^n. \tag{6.54}$$

The left-hand side of (6.54) is

$$\frac{1}{x}\left[G(x) - D_0\right] = \frac{1}{x}G(x) - \frac{1}{x}.$$

The second term on the right-hand side is

$$-\sum_{n=0}^{\infty}(-1)^n x^n = -\sum_{n=0}^{\infty}(-x)^n = -\frac{1}{1+x},$$

using the identity (6.42). Finally, the first term on the right-hand side can be rewritten as

$$\sum_{n=0}^{\infty} nD_n x^n + \sum_{n=0}^{\infty} D_n x^n = x\sum_{n=0}^{\infty} nD_n x^{n-1} + \sum_{n=0}^{\infty} D_n x^n = xG'(x) + G(x).$$

Thus, (6.54) becomes

$$\frac{1}{x}G(x) - \frac{1}{x} = xG'(x) + G(x) - \frac{1}{1+x},$$

or

$$G'(x) + (\frac{1}{x} - \frac{1}{x^2})G(x) = \frac{1}{x+x^2} - \frac{1}{x^2}. \tag{6.55}$$

Equation (6.55) is a linear first-order differential equation. Unfortunately, it is not easy to solve.

It turns out that the recurrence (6.53) is fairly easy to solve if we use instead of the ordinary generating function the exponential generating function

$$H(x) = \sum_{n=0}^{\infty} D_n \frac{x^n}{n!}.$$

To find $H(x)$, we multiply (6.53) by $x^{n+1}/(n+1)!$ and sum, obtaining

$$\sum_{n=0}^{\infty} D_{n+1}\frac{x^{n+1}}{(n+1)!} = \sum_{n=0}^{\infty}(n+1)D_n\frac{x^{n+1}}{(n+1)!} + \sum_{n=0}^{\infty}(-1)^{n+1}\frac{x^{n+1}}{(n+1)!}. \tag{6.56}$$

The left-hand side of (6.56) is

$$H(x) - D_0 = H(x) - 1.$$

The first term on the right-hand side is

$$\sum_{n=0}^{\infty} D_n \frac{x^{n+1}}{n!} = x\sum_{n=0}^{\infty} D_n \frac{x^n}{n!} = xH(x).$$

The second term on the right-hand side is

$$-\frac{x}{1!} + \frac{x^2}{2!} - \frac{x^3}{3!} + \cdots,$$

which is $e^{-x} - 1$ [see (5.3)]. Equation (6.56) now becomes

$$H(x) - 1 = xH(x) + e^{-x} - 1.$$

Hence,

$$H(x) = \frac{e^{-x}}{1-x}.$$

We may expand this out to obtain D_n, which is the coefficient of $x_n/n!$. Writing $H(x)$ as $e^{-x}(1-x)^{-1}$, we have

$$H(x) = \left[1 - x + \frac{x^2}{2!} - \frac{x^3}{3!} + \cdots\right]\left[1 + x + x^2 + \cdots\right]. \tag{6.57}$$

It is easy to see directly that

$$H(x) = \sum_{n=0}^{\infty} x^n \left[1 - \frac{1}{1!} + \frac{1}{2!} - \frac{1}{3!} + \cdots + (-1)^n \frac{1}{n!}\right],$$

so that the coefficient of $x^n/n!$ becomes

$$D_n = n!\left[1 - \frac{1}{1!} + \frac{1}{2!} - \frac{1}{3!} + \cdots + (-1)^n \frac{1}{n!}\right]. \tag{6.58}$$

Equation (6.58) agrees with our earlier formula (6.14).

Another way to derive D_n from $H(x)$ is to observe that $H(x)$ is the ordinary generating function of the sequence (c_n) which is the convolution of the sequences $((-1)^n/n!)$ and $(1, 1, 1, \ldots)$. Hence, $H(x)$ is the exponential generating function of $(n!c_n)$. Still a third way to derive D_n from $H(x)$ is explained in Exercise 20.

We close this subsection by deriving the recurrence (6.53). Note that, by (6.52),

$$\begin{aligned} D_{n+1} - (n+1)D_n &= D_{n+1} - nD_n - D_n \\ &= nD_{n-1} - D_n \\ &= -\left[D_n - nD_{n-1}\right]. \end{aligned}$$

Thus, we conclude that for all $j \geq 1$ and $k \geq 1$,

$$(-1)^j \left[D_j - jD_{j-1}\right] = (-1)^k \left[D_k - kD_{k-1}\right].$$

Now

$$(-1)^2 \left[D_2 - 2D_1\right] = 1\left[1 - 0\right] = 1.$$

Thus, we see that for $n \geq 0$,

$$(-1)^{n+1} \left[D_{n+1} - (n+1)D_n\right] = (-1)^2 \left[D_2 - 2D_1\right] = 1,$$

from which (6.53) follows for $n \geq 0$.

6.3.3 Simultaneous Equations for Generating Functions

In Section 6.1.4 we considered a situation where instead of one sequence, we had to use three sequences to find a satisfactory system of recurrences (6.19), (6.21), and (6.23). The method of generating functions can be applied to solve a system of recurrences. To illustrate, let us first choose a_0, b_0, and c_0 so that (6.19), (6.21), and (6.23) hold. Using $a_1 = 2, b_1 = 1, c_1 = 1$, we find from (6.19), (6.21), and (6.23) that

$$\begin{aligned} 2 &= 2a_0 + b_0 + c_0 \\ 1 &= b_0 - c_0 + 1 \\ 1 &= c_0 - b_0 + 1 \end{aligned}$$

One solution to this system is to take $a_0 = 1, b_0 = c_0 = 0$. With these values, we can assume that (6.19), (6.21), and (6.23) hold for $k \geq 0$.

We now multiply both sides of each of our equations by x^k and sum from $k = 0$ to ∞. We get

$$\begin{aligned} \sum_{k=0}^{\infty} a_{k+1}x^k &= 2\sum_{k=0}^{\infty} a_k x^k + \sum_{k=0}^{\infty} b_k x^k + \sum_{k=0}^{\infty} c_k x^k, \\ \sum_{k=0}^{\infty} b_{k+1}x^k &= \sum_{k=0}^{\infty} b_k x^k - \sum_{k=0}^{\infty} c_k x^k + \sum_{k=0}^{\infty} 4^k x^k, \\ \sum_{k=0}^{\infty} c_{k+1}x^k &= \sum_{k=0}^{\infty} c_k x^k - \sum_{k=0}^{\infty} b_k x^k + \sum_{k=0}^{\infty} 4^k x^k. \end{aligned}$$

If

$$A(x) = \textstyle\sum_{k=0}^{\infty} a_k x^k, \quad B(x) = \sum_{k=0}^{\infty} b_k x^k, \quad \text{and} \quad C(x) = \sum_{k=0}^{\infty} c_k x^k$$

are the ordinary generating functions for the sequences $(a_k), (b_k)$, and (c_k), respectively, we find that

$$\begin{aligned} \frac{1}{x}[A(x) - a_0] &= 2A(x) + B(x) + C(x), \\ \frac{1}{x}[B(x) - b_0] &= B(x) - C(x) + \frac{1}{1-4x}, \\ \frac{1}{x}[C(x) - c_0] &= C(x) - B(x) + \frac{1}{1-4x}. \end{aligned}$$

Using $a_0 = 1, b_0 = c_0 = 0$, we see from these three equations that

$$A(x) = \frac{1}{1-2x}\left[xB(x) + xC(x) + 1\right], \tag{6.59}$$

$$B(x) = \frac{1}{1-x}\left[-xC(x) + \frac{x}{1-4x}\right], \tag{6.60}$$

$$C(x) = \frac{1}{1-x}\left[-xB(x) + \frac{x}{1-4x}\right]. \tag{6.61}$$

It is easy to see from (6.60) and (6.61) that

$$B(x) = C(x) = \frac{x}{1-4x}. \tag{6.62}$$

It then follows from (6.59) and (6.62) that

$$A(x) = \frac{2x^2 - 4x + 1}{(1-2x)(1-4x)}. \tag{6.63}$$

By using (6.42), we see that (6.62) implies that

$$B(x) = C(x) = \sum_{k=0}^{\infty} 4^k x^{k+1}.$$

Thus, $b_k = c_k = 4^{k-1}$ for $k > 0$, $b_k = c_k = 0$ for $k = 0$. The right-hand side of (6.63) can be expanded out using the method of partial fractions, and we obtain

$$A(x) = \frac{1-3x}{1-4x} + \frac{x}{1-2x}.$$

This can be rewritten as

$$\begin{aligned} A(x) &= 1 + \frac{x}{1-4x} + \frac{x}{1-2x} \\ &= 1 + \sum_{k=0}^{\infty} 4^k x^{k+1} + \sum_{k=0}^{\infty} 2^k x^{k+1}. \end{aligned}$$

Thus, $a_k = 4^{k-1} + 2^{k-1}$ for $k > 0$, and $a_0 = 1$. The results can readily be checked. In particular, we have $a_2 = 4 + 2 = 6$, which agrees with the result obtained in Section 6.1.4.

EXERCISES FOR SECTION 6.3

Note to the reader: In each of these exercises, if the denominator of the generating function turns out to have complex roots, it is acceptable to give the generating function as the answer.

1. Use generating functions to solve the following recurrences.

   (a) (6.5) in Example 6.2 under the initial condition $f(1) = 0$

   (b) (6.6) in Example 6.3 (c) (6.7) in Example 6.3

2. Use generating functions to solve the following recurrences under the given initial conditions.

   (a) $a_{k+1} = a_k + 3, a_0 = 1$ (b) $a_{k+1} = 3a_k + 2, a_1 = 1$

   (c) $a_{k+2} = a_{k+1} - 2a_k, a_0 = 0, a_1 = 1$

3. Use generating functions to solve each of the recurrences in Exercise 12, Section 6.2.

4. In each of the following cases, suppose that $G(x)$ is the ordinary generating function for a sequence (a_k). Find a_k.

   (a) $G(x) = \dfrac{1}{(1-x)(1-3x)}$ (b) $G(x) = \dfrac{2x+1}{(1-3x)(1-2x)}$

   (c) $G(x) = \dfrac{2x^2}{(1-3x)(1-5x)(1-7x)}$ (d) $G(x) = \dfrac{1}{4x^2 - 5x + 1}$

   (e) $G(x) = \dfrac{x}{x^2 - 5x + 6}$ (f) $G(x) = \dfrac{1}{8x^3 - 6x^2 + x}$

5. Use the results of Section 6.3.3 to verify the values we obtained in Section 6.1.4 for:

   (a) a_3 (b) b_3 (c) c_3

6. Consider the product sales problem of Exercise 18, Section 6.1. Suppose that $A(x) = \sum_{n=0}^{\infty} a_n x^n$ is the ordinary generating function for (a_n).

   (a) If $a_0 = 0$ and $a_1 = 1$, find $A(x)$.

   (b) In general, find $A(x)$ in terms of a_0 and a_1.

   (c) If $a_0 = a_1$, use your answer to part (b) to show that a_n is constant. (This is obvious from the recurrence.)

7. In Exercise 21 of Section 6.1, find b_n.

8. This exercise asks the reader to derive the formula for the kth Fibonacci number by the method of generating functions.

   (a) It is useful to define F_{-1}. Use the recurrence (6.34) and the values of F_1 and F_0 to derive an appropriate value for F_{-1}.

   (b) If $G(x) = \sum_{k=0}^{\infty} F_k x^k$ is the ordinary generating function for F_k, derive a functional equation for $G(x)$ by multiplying the recurrence (6.34) by x^k and summing from $k = 0$ to ∞.

   (c) Show that
   $$G(x) = \frac{1}{1 - x - x^2}.$$

   (d) Find the roots of $1-x-x^2$ and use them to write $1-x-x^2$ as $(1-\lambda x)(1-\mu x)$.

   (e) Use partial fractions to write
   $$\frac{1}{(1-\lambda x)(1-\mu x)} \text{ as } \frac{A}{1-\lambda x} + \frac{B}{1-\mu x}.$$

   (f) From the result in part (e), derive a formula for F_k.

9. Suppose that G_n satisfies the equation
   $$G_{n+1} = G_n + G_{n-1},$$
   $n \geq 1$. Suppose that $G_0 = 3$ and $G_1 = 4$. Use generating functions to find a formula for G_n.

10. Use generating functions to solve the recurrence (6.10) in Example 6.7.

11. Solve the following recurrence:
    $$a_{k+1} = 2a_k + k + 5, \quad k \geq 0, \quad a_0 = 0.$$

12. Suppose that $a_{n+1} = (n+1)b_n$, for $n \geq 0$, and $a_0 = 0$. Find a relation involving $A(x), B'(x)$, and $B(x)$, if $A(x)$ and $B(x)$ are the ordinary generating functions for (a_n) and (b_n), respectively.

13. Suppose that
    $$y_{k+1} = Ay_k + B,$$
    for $k \geq 0$, where A and B are real numbers, $A \neq 1$. Find a formula for y_k in terms of y_0 using the method of generating functions.

14. Suppose that
$$y_{k+2} - y_{k+1} + 2y_k = 4^k,$$
$k \geq 0$, and that $y_0 = 2$, $y_1 = 1$. Find y_k using the method of generating functions.

15. Suppose that Y_t is national income at time t. Following Samuelson [1939], Goldberg [1958] derives the recurrence relation
$$Y_t = \alpha(1+\beta)Y_{t-1} - \alpha\beta Y_{t-2} + 1,$$
$t \geq 2$, for α and β positive constants. Assuming that $Y_0 = 2, Y_1 = 3, \alpha = \frac{1}{2}$, and $\beta = 1$, find a generating function for the sequence (Y_t).

16. Repeat Exercise 15 for $\alpha = 2$ and $\beta = 4$.

17. (Goldberg [1958]) In his work on inventory cycles, Metzler [1941] studies the total income i_t produced in the tth time period by an entrepreneur who is producing goods for sales and for inventory. Metzler derives the recurrence
$$i_{t+2} - 2\beta i_{t+1} + \beta i_t = v_0,$$
$t \geq 0$, where β is a constant such that $0 < \beta < 1$ and v_0 is a positive constant. Assuming that $i_0 = i_1 = 0$, find a generating function for the sequence (i_t).

18. If
$$C_{n+1} = 2nC_n + 2C_n + 2,$$
$n \geq 0$, and $C_0 = 1$, find C_n.

19. Solve the recurrence derived in Exercise 37, Section 6.1.

20. Derive D_n from Equation (6.57) for $H(x)$ by observing that $H(x)$ is the product of the exponential generating functions for the sequences (a_k) and (b_k), where $a_k = (-1)^k$ and $b_k = k!$. Use your results from Exercise 18, Section 5.5.

21. Derive a formula for D_n as follows.

    (a) Let
    $$C_n = \frac{D_n}{n!} - \frac{D_{n-1}}{(n-1)!}.$$
    Find a recurrence for C_{n+1} in terms of C_n.

    (b) Solve the recurrence for C_n by iteration.

    (c) Use the formula for C_n to solve for D_n.

22. Solve the recurrences of Exercise 22, Section 6.1, by the method of Section 6.3.3.

23. Solve simultaneously the recurrences
$$\begin{aligned} a_{n+1} &= a_n + b_n + c_n, \quad n \geq 1, \\ b_{n+1} &= 4^n - c_n, \quad n \geq 1, \\ c_{n+1} &= 4^n - b_n, \quad n \geq 1, \end{aligned}$$
subject to the initial conditions $a_1 = b_1 = c_1 = 1$.

24. (Anderson [1974]) Suppose that (a_n) satisfies
$$na_n = 2(a_{n-1} + a_{n-2}),$$
$n \geq 2$, and $a_0 = e, a_1 = 2e$. Let $A(x)$ be the ordinary generating function for (a_n).

(a) Show that $A'(x) = 2(1+x)A(x)$.

(b) Find $A(x)$. [*Hint:* Recall the equation $f'(x) = f(x)$.]

25. Consider a linear homogeneous recurrence relation (6.25) with constant coefficients. This exercise explores the relationship between the solution using characteristic roots and the solution using generating functions.

(a) Show that the ordinary generating function $G(x)$ for the sequence (a_n) is given by $G(x) = p(x)/q(x)$, where

$$q(x) = 1 - c_1 x - c_2 x^2 - \cdots - c_p x^p$$

and

$$\begin{aligned} p(x) &= a_0 + (a_1 - c_1 a_0)x + (a_2 - c_1 a_1 - c_2 a_0)x^2 + \cdots \\ &\quad + (a_{p-1} - c_1 a_{p-2} - \cdots - c_{p-1} a_0)x^{p-1}. \end{aligned}$$

(b) Show that if $\alpha_1, \alpha_2, \ldots, \alpha_p$ are the characteristic roots, then

$$q(x) = (1 - \alpha_1 x)(1 - \alpha_2 x) \cdots (1 - \alpha_p x)$$

and the roots of $q(x)$ are $1/\alpha_1, 1/\alpha_2, \ldots, 1/\alpha_p$.

(c) Illustrate these results by using the method of generating functions to solve the recurrence (6.29), and compare to the results in Section 6.2.1.

(d) Illustrate these results by using the method of characteristic roots to solve the recurrence (6.1), and compare to the results in Section 6.3.1.

26. Compute $R(x, B_J)$ for board B_J of Figure 5.6 by using Equation (6.50).

27. Compute the rook polynomial of board B in Figure 6.7 by using the results of Exercise 17 of Section 5.1, Example 5.14, and Equation (6.50).

6.4 SOME RECURRENCES INVOLVING CONVOLUTIONS[12]

6.4.1 The Number of Simple, Ordered, Rooted Trees

In Section 3.5.6 we noted that Cayley reduced the problem of counting the saturated hydrocarbons to the problem of counting trees. Here, we discuss a related problem, the problem of counting the number of *simple, ordered, rooted trees*, or *SOR trees* for short. These are (unlabeled) rooted trees[13] which are simple in the sense that each vertex has zero, one, or two children. Also, they are ordered so that the children of each vertex are labeled left (L) or right (R). We distinguish two SOR trees if they are not isomorphic, or if they have different roots, or if they have the same root and are isomorphic, but there is a disagreement on left or right children. For instance, the two SOR trees of Figure 6.8 are considered different even though they are isomorphic and have the same root.

[12] The four subsections of this section are relatively independent and can, in principle, be read in any order. From a purely pedagogical viewpoint, if there is not enough time for all four subsections, one of Sections 6.4.1, 6.4.2, 6.4.3 should be read—6.4.1 would be best—and then Section 6.4.4 should be read.

[13] For the definition of rooted tree, see Section 3.6.1.

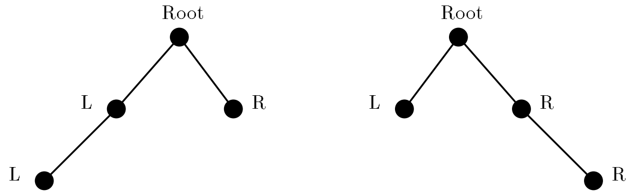

Figure 6.8: Two distinct SOR trees.

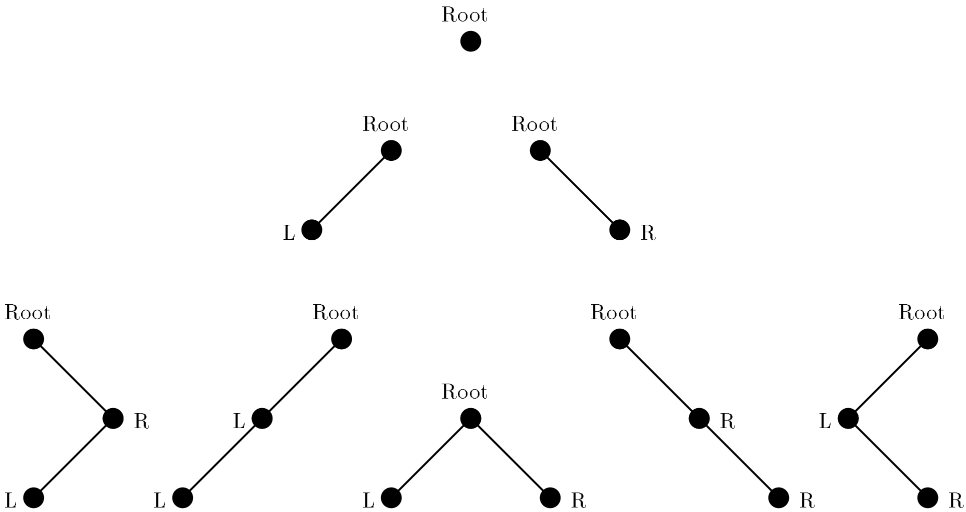

Figure 6.9: The distinct SOR trees of one, two, and three vertices.

We shall let u_n be the number of distinct SOR trees of n vertices. Then Figure 6.9 shows that $u_1 = 1, u_2 = 2$, and $u_3 = 5$. It is convenient to count the tree with no vertices as an SOR tree. Thus, we have $u_0 = 1$.

Suppose that T is an SOR tree of $n+1$ vertices, $n \geq 0$. Then the root has at most two children. If vertices a and b are the left and right children of the root in an SOR tree, then a and b themselves form the roots of SOR trees T_L and T_R, respectively. (If a or b does not exist, the corresponding SOR tree is the tree with no vertices.) In particular, if T_R has r vertices, T_L has $n-r$ vertices. Thus, we have the following recurrence:

$$u_{n+1} = u_0 u_n + u_1 u_{n-1} + u_2 u_{n-2} + \cdots + u_n u_0, \tag{6.64}$$

$n \geq 0$. Equation (6.64) gives us a way of computing u_{n+1} knowing all previous values u_i, $i \leq n$.

Note that the right-hand side of (6.64) comes from a convolution. In particular, if the sequence (v_n) is defined to be the sequence $(u_n) * (u_n)$, then

$$u_{n+1} = v_n. \tag{6.65}$$

Let $U(x) = \sum_{n=0}^{\infty} u_n x^n$ and $V(x) = \sum_{n=0}^{\infty} v_n x^n$ be the ordinary generating functions for the sequences (u_n) and (v_n), respectively. Then by (6.65),

$$\sum_{n=0}^{\infty} u_{n+1}x^n = \sum_{n=0}^{\infty} v_n x^n.$$

We conclude that

$$\frac{1}{x}\left[U(x) - u_0\right] = V(x),$$

so

$$\frac{1}{x}\left[U(x) - 1\right] = V(x). \tag{6.66}$$

But $V(x) = U(x)U(x) = U^2(x)$, so (6.66) gives us

$$xU^2(x) - U(x) + 1 = 0. \tag{6.67}$$

Equation (6.67) is a functional equation for $U(x)$. We can solve this functional equation by treating the unknown $U(x)$ as a variable y. Then, assuming that $x \neq 0$, we apply the quadratic formula to the equation

$$xy^2 - y + 1 = 0$$

and solve for y to obtain

$$y = U(x) = \frac{1 \pm \sqrt{1-4x}}{2x}. \tag{6.68}$$

We can now solve for u_n by expanding out. In particular, we note that $\sqrt{1-4x}$ can be expanded out using the binomial theorem (Theorem 5.3), giving us

$$\begin{aligned}(1-4x)^{1/2} &= 1 + \frac{1}{2}(-4x) + \frac{\frac{1}{2}\left(-\frac{1}{2}\right)}{2!}(-4x)^2 + \frac{\frac{1}{2}\left(-\frac{1}{2}\right)\left(-\frac{3}{2}\right)}{3!}(-4x)^3 + \\ &\quad \cdots + \binom{\frac{1}{2}}{r}(-4x)^r + \cdots.\end{aligned}$$

For $n \geq 1$, the coefficient of x^n here can be written as

$$\begin{aligned}
\binom{\frac{1}{2}}{n}(-4)^n &= \frac{\left(\frac{1}{2}\right)\left(-\frac{1}{2}\right)\left(-\frac{3}{2}\right)\cdots\left(\frac{1}{2}-n+1\right)}{n!}(-4)^n \\
&= \frac{\left(\frac{1}{2}\right)\left(-\frac{1}{2}\right)\left(-\frac{3}{2}\right)\cdots\left[-\frac{2n-3}{2}\right](-4)^n}{n!} \\
&= \frac{\left(\frac{1}{2}\right)(-1)^{n-1}\left(\frac{1}{2}\right)\left(\frac{3}{2}\right)\cdots\left[\frac{2n-3}{2}\right](-1)^n\,4^n}{n!} \\
&= \frac{\left(-\frac{1}{2^n}\right)[1\cdot 3\cdot 5\cdot\ldots\cdot(2n-3)]\,4^n}{n!} \\
&= \frac{-2^n\,[1\cdot 3\cdot 5\cdot\ldots\cdot(2n-3)]}{n!} \\
&= \frac{-2}{n}\frac{2^{n-1}}{(n-1)!}[1\cdot 3\cdot 5\cdot\ldots\cdot(2n-3)] \\
&= \frac{-2}{n}\frac{2^{n-1}\,[1\cdot 3\cdot 5\cdot\ldots\cdot(2n-3)]\,(n-1)!}{(n-1)!(n-1)!} \\
&= \frac{-2}{n}\frac{[1\cdot 3\cdot 5\cdot\ldots\cdot(2n-3)][2\cdot 4\cdot 6\cdot\ldots\cdot(2n-2)]}{(n-1)!(n-1)!} \\
&= \frac{-2}{n}\frac{(2n-2)!}{(n-1)!(n-1)!} \\
&= \frac{-2}{n}\binom{2n-2}{n-1}.
\end{aligned}$$

Thus,

$$(1-4x)^{1/2} = 1 - \sum_{n=1}^{\infty}\frac{2}{n}\binom{2n-2}{n-1}x^n. \tag{6.69}$$

Now (6.68) has two signs, that is, two possible solutions. If we take the solution of (6.68) with the $-$ sign, we have

$$U(x) = \frac{1}{2x}\left[1-\sqrt{1-4x}\right],$$

so

$$\begin{aligned}
U(x) &= \frac{1}{2x}\left[\sum_{n=1}^{\infty}\frac{2}{n}\binom{2n-2}{n-1}x^n\right], \\
&= \sum_{n=1}^{\infty}\frac{1}{n}\binom{2n-2}{n-1}x^{n-1},
\end{aligned}$$

$$= \sum_{n=0}^{\infty} \frac{1}{n+1}\binom{2n}{n} x^n, \tag{6.70}$$

by replacing n with $n+1$. We conclude from (6.70) that

$$u_n = \frac{1}{n+1}\binom{2n}{n}. \tag{6.71}$$

If we take the solution of (6.68) with the + sign, we find similarly that

$$U(x) = \frac{1}{x} - \sum_{n=1}^{\infty} \frac{1}{n}\binom{2n-2}{n-1} x^{n-1}, \tag{6.72}$$

so for $n \geq 1$,

$$u_n = -\frac{1}{n+1}\binom{2n}{n}. \tag{6.73}$$

Now the coefficients u_n must be nonnegative (why?), so (6.71) must be the solution, not (6.73). We also see that we must take the $-$ sign in (6.68) to get $U(x)$. We can see this directly from (6.72) also, since if $U(x)$ were given by (6.72), $U(x)$ would have a term $1/x$, yet $U(x) = \sum_{n=0}^{\infty} u_n x^n$.

The numbers u_n defined by (6.71) are called the *Catalan numbers*, after Eugene Charles Catalan. For instance, we find that

$$u_0 = \frac{1}{1}\binom{0}{0} = 1, \qquad u_1 = \frac{1}{2}\binom{2}{1} = 1, \qquad u_2 = \frac{1}{3}\binom{4}{2} = 2,$$

$$u_3 = \frac{1}{4}\binom{6}{3} = 5, \qquad u_4 = \frac{1}{5}\binom{8}{4} = 14.$$

The first four results agree with our earlier computations and the fifth can readily be verified. We shall see that the Catalan numbers are very common in combinatorics. See Eggleton and Guy [1988] for an extensive list of different contexts where the Catalan numbers appear.

6.4.2 The Ways to Multiply a Sequence of Numbers in a Computer

Suppose that we are given a sequence of n numbers, $x_1, x_2, \ldots, x_n$, and we wish to find their product. There are various ways in which we can find the product. For instance, suppose that $n = 4$. We can first multiply x_1 and x_2, then this product by x_3, and then this product by x_4. Alternatively, we can begin by multiplying x_1 and x_2, then multiply x_3 and x_4, and, finally, multiply the two products. We can distinguish these two and other approaches by inserting parentheses[14] as appropriate

[14] The parentheses do not distinguish between first performing x_1x_2, then x_3x_4, and multiplying the product, and first performing x_3x_4, then x_1x_2, and multiplying the product. We are only concerned with what products will have to be calculated.

in the string $x_1x_2\cdots x_n$. Thus, the first method corresponds to

$$(((x_1x_2)x_3)x_4)$$

and the second to

$$((x_1x_2)(x_3x_4)).$$

Let us assume that we must perform multiplications in the order given. For example, we do not allow multiplying x_1 by x_3 directly, and so on. Suppose that we are given a sequence of n numbers. How many different ways are there to instruct a computer to find the product? Suppose that P_n represents the number of ways in question. It is easy to see that finding the product corresponds to inserting $n-1$ left and $n-1$ right parentheses into the sequence $x_1x_2\cdots x_n$ in such a way that

1. one never has parentheses around a single term [i.e., (x_i) is not allowed], and
2. as we go from left to right, the number of right parentheses never exceeds the number of left parentheses.

Note that $P_1 = 1$, for there is only one way to insert 0 left and right parentheses. Also, $P_2 = 1, P_3 = 2$, and $P_4 = 5$. Table 6.4 demonstrates the parenthesizations corresponding to these numbers. It is easy to find a recurrence for P_n. Suppose that $n \geq 2$. Consider the last multiplication performed. This involves the product of two subproducts, $x_1\cdots x_r$ and $x_{r+1}\cdots x_n$. That is, we have for $1 < r < n-1$, the multiplication

$$((x_1\cdots x_r)(x_{r+1}\cdots x_n)).$$

If $r = 1$ or $n-1$, we have

$$(x_1(x_2\cdots x_n)) \quad \text{or} \quad ((x_1\cdots x_{n-1})x_n).$$

In either case, there are P_r ways to find the first subproduct and P_{n-r} ways to find the second subproduct, so we obtain the recurrence

$$P_n = \sum_{r=1}^{n-1} P_r P_{n-r}, \tag{6.74}$$

$n \geq 2$. Now if we let $P_0 = 0$, (6.74) becomes

$$P_n = \sum_{r=0}^{n} P_r P_{n-r}, \tag{6.75}$$

$n \geq 2$. Now let $P(x) = \sum_{n=0}^{\infty} P_n x^n$ be the ordinary generating function for the sequence (P_n). Equation (6.75) suggests that (P_n) is related to the convolution $(P_n) * (P_n)$. However, since (6.75) holds only for $n \geq 2$, we cannot conclude that $P(x) = P^2(x)$. To get around this difficulty, we define the sequence (Q_n) to be the sequence $(P_n) * (P_n)$. Then note that

$$Q_n = \begin{cases} 0 = P_0P_0 & \text{if } n = 0 \\ 0 = P_0P_1 + P_1P_0 & \text{if } n = 1 \\ P_n & \text{if } n \geq 2 \end{cases} \tag{6.76}$$

Table 6.4: The Ways of Performing a Multiplication of Two, Three, or Four Numbers

P_2	P_3	P_4
(x_1x_2)	$((x_1x_2)x_3)$	$(((x_1x_2)x_3)x_4)$
	$(x_1(x_2x_3))$	$(x_1(x_2(x_3x_4)))$
		$((x_1(x_2x_3))x_4)$
		$(x_1((x_2x_3)x_4))$
		$((x_1x_2)(x_3x_4))$

and the ordinary generating function $Q(x) = \sum_{n=0}^{\infty} Q_n x^n$ satisfies

$$Q(x) = P^2(x).$$

Moreover, by (6.76),

$$Q(x) = P(x) - x,$$

since $P_n = Q_n$ for $n \neq 1$, and $P_1 = 1, Q_1 = O$. Thus, we know that

$$P(x) - x = P^2(x).$$

This is a functional equation for P(x). We solve it by rewriting it as a quadratic in the unknown $y = P(x)$ and using the quadratic formula, obtaining

$$P^2(x) - P(x) + x = 0,$$

$$P(x) = \frac{1 \pm \sqrt{1-4x}}{2}. \tag{6.77}$$

To find P_n, we could expand out $P(x)$ using the binomial theorem. Alternatively, we recognize that $P(x)$ is $xU(x)$ for $U(x)$ of (6.68). Thus, $P_n = u_{n-1}$ for $n \geq 1$. We have defined $P_0 = 0$. By formula (6.71), we find that for $n \geq 1$,

$$P_n = \frac{1}{n}\binom{2n-2}{n-1}. \tag{6.78}$$

The Catalan numbers have shown up again.

The close relation between the numbers u_n and P_n suggests that we might be able to find a direct relationship between SOR trees and order of multiplication. Following Even [1973], we shall describe such a relationship. Let us consider just a sequence of n left and n right parentheses. Such a sequence is called *well-formed* if condition 2 above holds. Let K_n be the number of such sequences. Then clearly $P_n = K_{n-1}$. Given an SOR tree of n vertices, associate with each vertex of degree 1 the sequence of parentheses ( ). Associate with every other vertex the following sequence: (, followed by the sequence associated with its left child (if there is one),

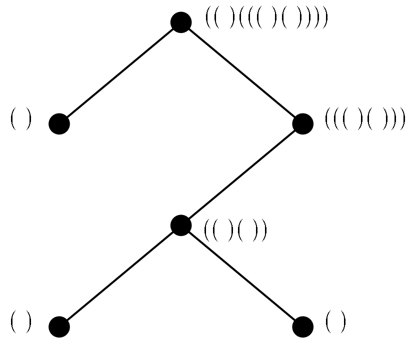

Figure 6.10: Next to each vertex is the corresponding well-formed sequence of parentheses.

followed by the sequence associated with its right child (if there is one), followed by). This associates a unique well-formed sequence of parentheses with each SOR tree, the sequence assigned to its root. Figure 6.10 illustrates the procedure. Conversely, given a well-formed sequence of n left and n right parentheses, one can show that it comes from an SOR tree of n vertices. This is left as an exercise (Exercise 17). Thus, $K_n = u_n$, and we again have the conclusion $P_n = u_{n-1}$.

6.4.3 Secondary Structure in RNA

In Sections 2.11 and 2.12 we studied the linear chain of bases in an RNA molecule. This chain is sometimes said to define the *primary structure* of RNA. When RNA has only the bonds between neighbors in the chain, it is said to be a *random coil.* Now RNA does not remain a random coil. It folds back on itself and forms new bonds referred to as *Watson-Crick bonds*, creating helical regions. In such Watson-Crick bonding of an RNA chain $s = s_1s_2\cdots s_n$, each base can be bonded to at most one other nonneighboring base and if s_i and s_j are bonded, and $i < k < j$, then s_k can only be bonded with bases between s_{i+1} and s_{j-1}; that is, there is no crossover.[15] The new bonds define the *secondary structure* of the original RNA chain. Figure 6.11 shows one possible secondary structure for the RNA chain

AACGGGCGGGACCCUUCAACCCUU.

Watson-Crick bonds usually form between A and U bases or between G and C bases, but we shall, following Howell, Smith, and Waterman [1980], find it convenient to allow all possible bonds in our discussion. In studying RNA chains, Howell, Smith, and Waterman [1980] use recurrences to compute the number R_n of possible secondary structures for an RNA chain of length n. We briefly discuss their approach.[16] For more on secondary structure, see Clote and Backofen [2000], Setubal and Meidanis [1997], and Waterman [1995].

[15] For a related bonding problem, see Nussinov, *et al.* [1978].
[16] For related work, see Stein and Waterman [1978] and Waterman [1978].

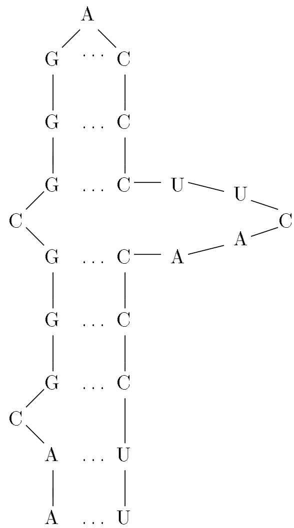

Figure 6.11: A secondary structure for the RNA chain AACGGGCGGGA-CCCUUCAACCCUU. The Watson-Crick bonds are dotted. (Reproduced from Howell, Smith, and Waterman [1980]. Copyright ©1980 Society for Industrial and Applied Mathematics. Reprinted with permission. All rights reserved.)

Note that $R_1 = R_2 = 1$, for there can be no Watson-Crick bonds. Also, $R_0 = 1$ by convention. Consider an RNA chain $s_1 s_2 \cdots s_{n+1}$ of length $n+1 \geq 3$. Now either s_{n+1} is not Watson-Crick bonded, or it is bonded with s_j, $1 \leq j \leq n-1$. Thus, for $n \geq 2$,

$$R_{n+1} = R_n + \sum_{j=1}^{n-1} R_{j-1} R_{n-j}, \tag{6.79}$$

since in the first case, the chain $s_1 s_2 \cdots s_n$ is free to form any secondary structure, and in the second case, the subchains $s_1 s_2 \cdots s_{j-1}$ and $s_{j+1} s_{j+2} \cdots s_n$ are free to form any secondary structure. This is a recurrence for R_n. Let $R(x)$ be the ordinary generating function for R_n, that is,

$$R(x) = \sum_{n=0}^{\infty} R_n x^n.$$

To find $R(x)$, we note that the second term on the right-hand side of (6.79) almost arises from a convolution. If we define $(T_n) = (R_n) * (R_n)$, and we use the fact that $R_0 = 1$, we have for $n \geq 2$,

$$R_{n+1} = R_n + \sum_{j=1}^{n} R_{j-1} R_{n-j} - R_{n-1} R_0,$$

and hence for $n \geq 2$,

$$R_{n+1} = R_n - R_{n-1} + T_{n-1}. \tag{6.80}$$

It is easy to see that (6.80) still holds for $n = 1$. Furthermore, if we define $R_{-1} = T_{-1} = 0$, (6.80) holds for all $n \geq 0$. Now let $T(x) = \sum_{n=0}^{\infty} T_n x^n$ be the ordinary generating function for (T_n). By (6.80),

$$\sum_{n=0}^{\infty} R_{n+1}x^n = \sum_{n=0}^{\infty} R_n x^n - \sum_{n=0}^{\infty} R_{n-1}x^n + \sum_{n=0}^{\infty} T_{n-1}x^n.$$

Hence,

$$\frac{1}{x}\left[R(x) - R_0\right] = R(x) - x\left[\frac{R_{-1}}{x} + R(x)\right] + x\left[\frac{T_{-1}}{x} + T(x)\right],$$

so

$$\frac{1}{x}[R(x) - 1] = R(x) - xR(x) + xT(x).$$

Since (T_n) is a convolution of (R_n) with itself,

$$T(x) = R^2(x).$$

Thus, we have

$$\frac{1}{x}R(x) - \frac{1}{x} = R(x) - xR(x) + xR^2(x),$$

or

$$x^2R^2(x) + (-x^2 + x - 1)R(x) + 1 = 0.$$

We find, for $x \neq 0$,

$$R(x) = \frac{x^2 - x + 1 \pm \sqrt{(-x^2 + x - 1)^2 - 4x^2}}{2x^2},$$

or

$$R(x) = \frac{1}{2x^2}\left[x^2 - x + 1 \pm \sqrt{1 - (2x + x^2 + 2x^3 - x^4)}\right]. \tag{6.81}$$

The square root in (6.81) can be expanded using the binomial theorem. Note that we can easily determine whether the + or $-$ sign is to be used in (6.81) by noting that if the + sign is used, there is a term $1/2x^2$. Thus, the $-$ sign must be right. We can also see this by considering what happens as x approaches 0. Now $R(x)$ should approach $R(0) = R_0 = 1$. If we use the + sign in (6.81), $R(x)$ approaches ∞ as x approaches 0. Thus, the $-$ sign must be right.

6.4.4 Organic Compounds Built Up from Benzene Rings

Harary and Read [1970] and Anderson [1974] point out that certain organic compounds built up from benzene rings can be represented by a configuration of hexagons, as for example in Figure 6.12. Counting hexagonal configurations of various kinds is a central topic in mathematical chemistry. (For a survey of this topic, see

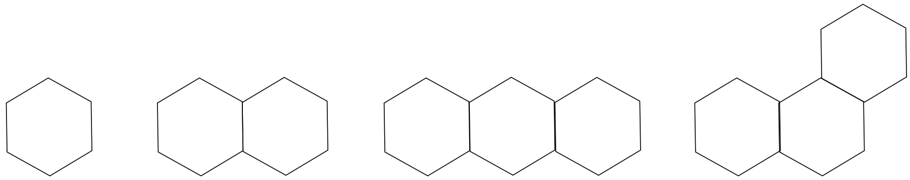

Figure 6.12: Some organic compounds built up from benzene rings.

Cyvin, Brunvoll, and Cyvin [1992].) We illustrate the idea with a counting method using generating functions.

We shall be interested in *polyhexes*, configurations of hexagons in which all hexagons are congruent, regular hexagons, any two such hexagons are either disjoint or share a common edge, and the configuration is connected if we think of it as a graph. We add the restriction that no three hexagons can meet at a point. Then we get *catacondensed polyhexes*.

Following Harary and Read [1970], we consider only catacondensed polyhexes generated by starting with a catacondensed polyhex and adding one hexagon at one of the edges along the "perimeter" of the polyhex. In particular, we make the simplifying assumption that all polyhexes are generated starting from a base hexagon with a base edge as shown in Figure 6.13. Onto this base, one can attach a hexagon only at the sides labeled 1, 2, and 3. Thus, by our previous assumptions, one cannot attach a hexagon at both edge 1 and 2 or at both edge 2 and 3. Let us call a catacondensed polyhex constructed this way with n hexagons in all a *polyhexal configuration*, or an *n-polyhex* for short. In general, an n-polyhex (a polyhex of n hexagons) is obtained from an $(n-1)$-polyhex by attaching a new hexagon to one of the edges of the $(n-1)$-polyhex. This nth hexagon and the $(n-1)$-polyhex can only have a single edge in common. Let h_k denote the number of possible k-polyhexes. We wish to compute h_k. Rather than derive a recurrence for h_k directly, we introduce two other sequences and use these to compute h_k. Let s_k denote the number of such configurations where only one hexagon is joined to the base, and d_k denote the number where exactly two hexagons are joined to the base. Obviously,

$$h_k = s_k + d_k, \tag{6.82}$$

$k \geq 2$. However, (6.82) fails for $k = 1$, since $h_1 = 1$ and $s_1 = d_1 = 0$. If we have a $(k+1)$-polyhex and only one hexagon is joined to the base, there are three possible edges on which to join it, so

$$s_{k+1} = 3h_k, \tag{6.83}$$

$k \geq 1$. If we have a $(k+1)$-polyhex and two hexagons are joined to the base, they must use edges 1 and 3 of Figure 6.13, since three hexagons may not meet in a point. Thus, a r-polyhex is joined to edge 1 and a $k-r$-polyhex is joined to edge 3, with $1 \leq r \leq k-1$. We conclude that

$$d_{k+1} = h_1 h_{k-1} + h_2 h_{k-2} + \cdots + h_{k-1} h_1 \tag{6.84}$$

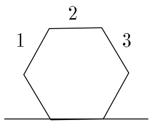

Figure 6.13: A base hexagon.

for $k \geq 2$. Note that the three recurrences (6.82), (6.83), and (6.84) can be used together to compute the desired numbers h_k iteratively. Knowing $h_1, h_2, \ldots, h_k$, we use (6.83) and (6.84) to compute s_{k+1} and d_{k+1}, respectively, and then obtain h_{k+1} from (6.82). This situation is analogous to the situation in Section 6.1.4, where we first encountered a system of recurrences.

Consider now the ordinary generating functions

$$H(x) = \sum_{k=0}^{\infty} h_k x^k, \quad S(x) = \sum_{k=0}^{\infty} s_k x^k, \quad D(x) = \sum_{k=0}^{\infty} d_k x^k. \tag{6.85}$$

We shall compute $H(x)$. The technique for finding it will be somewhat different from that in the previous subsections. It will make use of the results of Section 5.2 on operating on generating functions. Note that h_k, s_k, and d_k are all defined only from $k = 1$ to ∞. To use the generating functions of (6.85), it is convenient to define $h_0 = s_0 = d_0 = 0$ and so to be able to take the sums from 0 to ∞. If we take $h_0 = s_0 = d_0 = 0$, then (6.82) holds for $k = 0$ as well as $k \geq 2$. Also, since $s_1 = 0$ and $h_0 = 0$, (6.83) now holds for all $k \geq 0$. Since $h_0 = 0$, we can add $h_0 h_k + h_k h_0$ to the right-hand side of (6.84), obtaining

$$d_{k+1} = h_0 h_k + h_1 h_{k-1} + h_2 h_{k-2} + \cdots + h_k h_0, \tag{6.86}$$

for all $k \geq 2$. But it is easy to see that (6.86) holds for all $k \geq 0$, since $d_1 = 0 = h_0 h_0$ and $d_2 = 0 = h_0 h_1 + h_1 h_0$.

Using (6.82), we are tempted to conclude, by the methods of Section 5.2, that

$$H(x) = S(x) + D(x).$$

However, this is not true since (6.82) is false for $k = 1$. If we define

$$g_k = \begin{cases} h_k & \text{if } k \neq 1 \\ 0 & \text{if } k = 1, \end{cases}$$

then

$$g_k = s_k + d_k$$

holds for all $k \geq 0$. Moreover, if

$$G(x) = \sum_{k=0}^{\infty} g_k x^k,$$

then

$$G(x) = S(x) + D(x).$$

Finally,

$$H(x) = G(x) + x \tag{6.87}$$

since the sequence (h_k) is the sum of the sequence (g_k) and the sequence (0, 1, 0, 0, ...). Thus,

$$H(x) = S(x) + D(x) + x. \tag{6.88}$$

Next, we have observed that (6.83) holds for $k \geq 0$. Hence,

$$\sum_{k=0}^{\infty} s_{k+1} x^k \; = \; 3 \sum_{k=0}^{\infty} h_k x^k,$$

or

$$\frac{1}{x}\left[S(x) - s_0\right] = 3H(x),$$

and since $s_0 = 0$,

$$\frac{1}{x} S(x) = 3H(x).$$

Thus,

$$S(x) = 3xH(x). \tag{6.89}$$

Finally, let us simplify $D(x)$. Letting $e_k = d_{k+1}, k \geq 0$, we see from (6.86) that (e_k) is the convolution of the sequence (h_k) with itself. Letting

$$E(x) = \sum_{k=0}^{\infty} e_k x^k,$$

we have

$$E(x) = H^2(x). \tag{6.90}$$

Then

$$\begin{aligned} D(x) &= \sum_{k=0}^{\infty} d_k x^k &&= \sum_{k=1}^{\infty} d_k x^k \\ &= \sum_{k=1}^{\infty} e_{k-1} x^k &&= x \sum_{k=1}^{\infty} e_{k-1} x^{k-1} \\ &= x \sum_{k=0}^{\infty} e_k x^k &&= xE(x). \end{aligned}$$

Thus, by (6.90),

$$D(x) = xH^2(x). \tag{6.91}$$

Using (6.89) and (6.91) in (6.88) gives

$$H(x) = 3xH(x) + xH^2(x) + x,$$

or

$$xH^2(x) + (3x - 1)H(x) + x = 0. \tag{6.92}$$

Equation (6.92) is a quadratic equation for the unknown function $H(x)$. We solve it by the quadratic formula, obtaining

$$H(x) = \frac{1}{2x}\left[1 - 3x \pm \sqrt{(3x-1)^2 - 4x^2}\right]$$

or

$$H(x) = \frac{1}{2x}\left[1 - 3x \pm \sqrt{1 - (6x - 5x^2)}\right], \tag{6.93}$$

$x \neq 0$. $H(x)$ can be expanded out using the binomial theorem, and the proper sign, $+$ or $-$, can be chosen once the expansion has been obtained.

The method we have described for computing h_k is, unfortunately, flawed. It is possible to use the method of building up to a k-polyhex that we have described and end up with a configuration which has three hexagons meeting at a point, i.e., that violates the catacondensed condition. (Verification of this fact is left to the reader as an exercise; see Exercise 23.) A second complication of the method we have described is that it can give rise to configurations that circle around and return to themselves in a *ring* that encloses somewhere inside it a hexagon not part of the configuration. One can also end up with hexagons that overlap other than along edges. (Verification of these two additional complications are also left to the reader as exercises; see Exercise 23.) Thus, while the counting method we have described is clever, it overestimates the number of k-polyhexes and it counts configurations such as rings that are not satisfactory. Harary and Read knew about the problems of the type we have described. They rationalized the violation of the no three hexagons meeting at a point property and the property that hexagons overlap only along common edges by thinking of the configuration as broken up into layers, with the system at some point passing from one layer to another. Thus, once a configuration of hexagons circles back on itself to create a ring or a situation of three hexagons meeting at a point, we think of it as taking off in another dimension and lying on top of a previous part of the configuration and overlapping it. This is now a standard idea in the literature (see Cyvin, Brunvoll, and Cyvin [1992]).

The difficulties we have observed illustrate the fact that the use of generating functions or any other method to get an exact count of hexagonal configurations has not met with total success. For the most part, computer-generated methods have replaced generating functions for counting various kinds of configurations. Knop, *et al.* [1983] were the first to publish results of this type for k-polyhexes, $k \leq 10$. Further advances continue to be made; see, for example, Tošić, *et al.* [1995].

EXERCISES FOR SECTION 6.4

1. Check that the Catalan number $u_4 = 14$ does indeed count the number of SOR trees of four vertices.
2. Compute the Catalan numbers u_5 and u_6.

3. Use (6.78) to compute P_5 and check that it does indeed count the number of ways to multiply a sequence of 5 numbers.
4. Compute R_3, R_4, and R_5 from the recurrence (6.79) and the initial conditions, and check by drawing the appropriate secondary structures.
5. Compute h_2, h_3, and h_4 from the recurrences (6.82)–(6.84) and the initial conditions, and check your answers by drawing the appropriate polyhexes.
6. When generating n-polyhexes, if we remove the assumption that the nth hexagon and $(n-1)$-polyhex can only have a single edge in common, then rings can form and internal "holes" can be formed in the polyhex. If there is exactly one hole and it has the size of one hexagon, the polyhex is called a *circulene*.

   (a) What is the smallest number of hexagons needed to form a circulene?

   (b) What is the smallest number of hexagons needed to form a polyhex with a hole at least the size of two hexagons? (Such a polyhex is called a *coronoid*.)

   (c) What is the smallest number of hexagons needed to form a coronoid with two holes each with size at least two hexagons?

7. A *rooted tree* is called *ordered* if a fixed ordering from left to right is assigned to all the children of a given vertex. Put another way, the k children of a given vertex are labeled with the integers $1, 2, \ldots, k$. Two rooted, ordered trees are considered different if they are not isomorphic or if they have a different root or if they are isomorphic and have the same root, but the order of children of two associated vertices differs. Suppose that r_n is the number of rooted, ordered trees of n vertices and $r_n(k)$ is the number of rooted, ordered trees of n vertices where the root has degree k.

   (a) Find an expression for r_n in terms of the $r_n(k)$.

   (b) Find an expression for $r_n(2)$ in terms of the other r_n's.

8. Suppose that

$$A(x) = \textstyle\sum_{n=0}^{\infty} a_n x^n, \quad B(x) = \sum_{n=0}^{\infty} b_n x^n, \quad \text{and} \quad C(x) = \sum_{n=0}^{\infty} c_n x^n$$

   are the ordinary generating functions for the sequences $(a_n), (b_n)$, and (c_n), respectively. Suppose that $a_0 = b_0 = c_0 = 0, a_1 = c_1 = 0, b_1 = 1$, and $a_2 = b_2 = 0, c_2 = 1$.

   (a) Suppose that $c_n = a_n + b_n, n \geq 3$. Translate this into a statement in terms of generating functions.

   (b) Suppose that $a_{n+1} = 4c_n, n \geq 0$. Translate this into a statement in terms of generating functions.

   (c) Suppose that $b_{n+1} = c_1 c_{n-1} + c_2 c_{n-2} + \cdots + c_{n-1} c_1, n \geq 2$. Translate this into a statement using generating functions.

   (d) Use your answers to parts (a)–(c) to derive an equation involving only $C(x)$.

9. Suppose that $A(x), B(x), C(x), a_0, b_0, c_0, a_1, b_1, c_1, a_2$, and b_2 are as in Exercise 8, and $c_2 = 4$.

   (a) Suppose that $c_n = a_n + 2b_n + 2, n \geq 3$. Translate this into a statement using generating functions.

(b) Suppose that $a_{n+1} = 3c_n, n \geq 0$. Translate this into a statement using generating functions.

(c) Suppose that $b_{n+1} = c_1c_{n-1} + c_2c_{n-2} + \cdots + c_{n-1}c_1, n \geq 2$. Translate this into a statement using generating functions.

(d) Use your answers to parts (a)–(c) to derive an equation involving only $C(x)$.

10. If $H(x)$ is given by (6.93), how can you tell whether to use the + sign or the − sign in computing $H(x)$?

11. (a) Use the formula for $H(x)$ [Equation (6.93)] to compute the number h_1.

(b) Repeat for h_2. (c) Repeat for h_3.

12. Prove that the Catalan numbers $u_n = \dfrac{1}{n+1}\dbinom{2n}{n}$, $n = 0, 1, 2, \ldots$, are integers by finding two binomial coefficients whose difference is u_n. $\left[\textit{Hint:} \text{ Consider } \dbinom{2n}{n}.\right]$

13. (Waterman [1978]) This exercise will find a lower bound for R_n, the number of possible secondary structures for an RNA chain of length n.

(a) Show from Equation (6.79) and the initial conditions that for $n \geq 2$,

$$R_{n+1} = R_n + R_{n-1} + \sum_{k=1}^{n-2} R_k R_{n-k-1}. \tag{6.94}$$

(b) By using Equation (6.94) and the equation obtained by replacing $n+1$ by n in (6.94), show from the initial conditions that for $n \geq 2$,

$$R_{n+1} = R_n + R_{n-1} + R_{n-2} + \sum_{k=1}^{n-3} R_k R_{n-k-1}. \tag{6.95}$$

(c) Since $R_{p+1} \geq R_p$, conclude that for $n \geq 2$, $R_{n+1} \geq 2R_n$, and so for $n \geq 2$, $R_n \geq 2^{n-2}$.

14. (Riordan [1975]) Suppose that $2n$ points are arranged on the circumference of a circle. Pair up these points and join corresponding points by chords of the circle. Show that the number C_n of ways of doing this pairing so that none of the chords cross is given by a Catalan number. (Maurer [1992] and Nussinov, *et al.* [1978] relate intersection patterns of these chords to biochemical problems, and Ko [1979], Read [1979], and Riordan [1975] study the number of ways to obtain exactly k overlaps of the chords.)

15. (Even [1973]) A *Last In-First Out* (LIFO) *stack* is a memory device that is like the stack of trays in a cafeteria: The last tray put on top of the stack is the first one that can be removed. A sequence of items labeled $1, 2, \ldots, n$ is waiting to be put into an empty LIFO stack. It must be put into the stack in the order given. However, at any time, we may remove an item. Removed items are never returned to the stack or the sequence awaiting storage. At the end, we remove all items from the stack and achieve a permutation of the labels $1, 2, \ldots, n$. For instance, if $n = 3$, we can first put in 1, then put in 2, then remove 2, then remove 1, then put in 3, and, finally, remove 3, obtaining the permutation $2, 1, 3$. Let q_n be the number of permutations attainable.

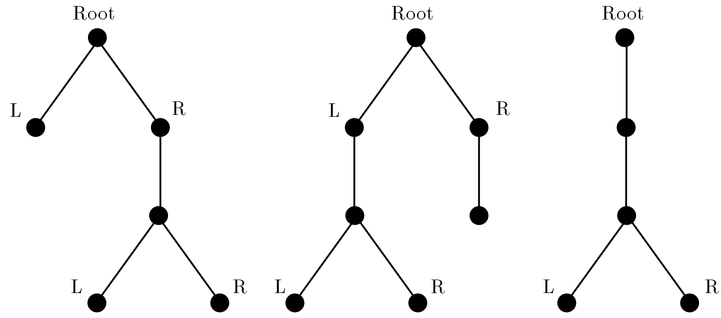

Figure 6.14: Several SPR trees.

(a) Find q_1, q_2, q_3, and q_4.

(b) Find q_n by obtaining a recurrence and solving.

16. In Section 6.4.4, suppose that we take $h_0 = -\frac{3}{2}$ instead of $h_0 = 0$.[17]

(a) Show that
$$h_{k+1} = h_0 h_k + h_1 h_{k-1} + \cdots + h_k h_0$$
holds for all $k \geq 2$.

(b) Define (c_k) to be the sequence $(h_k) * (h_k)$ and let $w_k = h_{k+1}$. Let $C(x)$ be the ordinary generating function for (c_k) and $W(x)$ be the ordinary generating function for (w_k). Relate $W(x)$ and $C(x)$ to $H(x)$ and derive a functional equation for $H(x)$.

(c) Solve for $H(x)$.

(d) Why is the answer in part (c) different from the formula for $H(x)$ given in (6.93)? What is the relation of the new $H(x)$ to the old $H(x)$?

17. Show that each well-formed sequence of n left and n right parentheses comes from some SOR tree by the method described in Section 6.4.2.

18. Let v_n count the number of ways n votes can come in for each of two candidates A and B in an election, where A never trails B. Find v_n by exhibiting a direct relationship between these orders of votes and the orders of multiplication of n numbers.

19. (Anderson [1974]) A *simple, partly ordered, rooted tree* (SPR *tree*) is a simple rooted tree in which the labels L and R are placed on the children of a vertex only if there are two children. Figure 6.14 shows several SPR trees. Let u_n count the number of SPR trees of n vertices, let a_n count the number of SPR trees of n vertices in which the root has one child, and let b_n count the number of SPR trees of n vertices in which the root has two children. Assume that $a_0 = b_0 = u_0 = 0$. Let $U(x)$, $A(x)$, and $B(x)$ be the ordinary generating functions for (u_n), (a_n), and (b_n), respectively.

(a) Compute a_1, b_1, u_1, a_2, b_2, and u_2.

[17] This idea is due to Martin Farber [personal communication].

(b) Derive a relation that gives u_n in terms of a_n and b_n and holds for all $n \neq 1$.

(c) Derive a relation that gives a_{n+1} in terms of u_n and holds for all $n \geq 0$.

(d) Derive a relation that gives b_{n+1} in terms of $u_1, u_2, \ldots, u_n$, and holds for all $n \geq 2$.

(e) Derive a relation that gives b_{n+1} in terms of $u_0, u_1, u_2, \ldots, u_n$, and holds for all $n \geq 0$.

(f) Find u_3, u_4, a_3, a_4, b_3, and b_4 from the answers to parts (b), (c), and (e), and check by drawing SPR trees.

(g) Translate your answer to part (b) into a statement in terms of generating functions.

(h) Do the same for part (c).

(i) Do the same for part (e).

(j) Show that

$$U(x) = \frac{1}{2x}\left[1 - x \pm \sqrt{(x-1)^2 - 4x^2}\right].$$

20. (Liu [1968]) Suppose that $A(x)$ is the ordinary generating function for the sequence (a_n) and $B(x)$ is the ordinary generating function for the sequence (b_n), and that

$$b_n = a_{n-1}b_0 + a_{n-2}b_1 + \cdots + a_0 b_{n-1}, \quad n \geq 1.$$

Find a relation involving $A(x)$ and $B(x)$.

21. Generalize the result in Exercise 20 to the case

$$b_n = a_{n-r}b_0 + a_{n-r-1}b_1 + \cdots + a_0 b_{n-r}$$

for $n \geq k$, where $k \geq r$.

22. (Liu [1968]) Recall the definition of pattern in a bit string introduced in Exercise 37, Section 6.1. Let a_n be the number of n-digit bit strings that have the pattern 010 occurring for the first time at the nth digit.

(a) Show that

$$2^{n-3} = a_n + a_{n-2} + a_{n-3}2^0 + a_{n-4}2^1 + \cdots + a_3 2^{n-6},$$

$n \geq 6$.

(b) Let $b_0 = 1, b_1 = 0, b_2 = 1, b_3 = 2^0, b_4 = 2^1, b_5 = 2^2, \ldots$, and let $a_0 = a_1 = a_2 = 0$. Show that

$$2^{n-3} = a_n b_0 + a_{n-1}b_1 + a_{n-2}b_2 + \cdots + a_0 b_n,$$

$n \geq 3$.

(c) Letting $A(x)$ and $B(x)$ be the ordinary generating functions for the sequences (a_n) and (b_n), respectively, translate the equation obtained in part (b) into a statement involving $A(x)$ and $B(x)$. (See Exercise 21.)

(d) Solve for $A(x)$.

23. Show that it is possible, using the method of building up to a k-polyhex that we have described in Section 6.4.4, to end up with a configuration that:

(a) Has three hexagons meeting at a point, i.e., that violates the catacondensed condition

(b) Circles around and returns to itself in a ring that encloses somewhere inside it a hexagon not part of the configuration

(c) Has hexagons that overlap other than along edges

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