Discrete Math for Computer Science Students

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Contents

Chapter 1

Counting

1.1 Basic Counting

The Sum Principle

We begin with an example that illustrates a fundamental principle.

Exercise 1.1-1 The loop below is part of an implementation of selection sort, which sorts a list of items chosen from an ordered set (numbers, alphabet characters, words, etc.) into non-decreasing order.

```
(1)  for i = 1 to n − 1
(2)       for j = i + 1 to n
(3)            if (A[i] > A[j])
(4)                 exchange A[i] and A[j]
```

How many times is the comparison $A[i] > A[j]$ made in Line 3?

In Exercise 1.1-1, the segment of code from lines 2 through 4 is executed $n-1$ times, once for each value of i between 1 and $n-1$ inclusive. The first time, it makes $n-1$ comparisons. The second time, it makes $n-2$ comparisons. The ith time, it makes $n-i$ comparisons. Thus the total number of comparisons is

$$(n-1) + (n-2) + \cdots + 1 \; . \tag{1.1}$$

This formula is not as important as the reasoning that lead us to it. In order to put the reasoning into a broadly applicable format, we will describe what we were doing in the language of sets. Think about the set S containing all comparisons the algorithm in Exercise 1.1-1 makes. We divided set S into $n-1$ pieces (i.e. smaller sets), the set S_1 of comparisons made when $i = 1$, the set S_2 of comparisons made when $i = 2$, and so on through the set S_{n-1} of comparisons made when $i = n-1$. We were able to figure out the number of comparisons in each of these pieces by observation, and added together the sizes of all the pieces in order to get the size of the set of all comparisons.

in order to describe a general version of the process we used, we introduce some set-theoretic terminology. Two sets are called *disjoint* when they have no elements in common. Each of the sets S_i we described above is disjoint from each of the others, because the comparisons we make for one value of i are different from those we make with another value of i. We say the set of sets $\{S_1, \ldots, S_m\}$ (above, m was $n-1$) is a family of *mutually disjoint sets*, meaning that it is a family (set) of sets, any two of which are disjoint. With this language, we can state a general principle that explains what we were doing without making any specific reference to the problem we were solving.

Principle 1.1 (Sum Principle) *The size of a union of a family of mutually disjoint finite sets is the sum of the sizes of the sets.*

Thus we were, in effect, using the sum principle to solve Exercise 1.1-1. We can describe the sum principle using an algebraic notation. Let $|S|$ denote the size of the set S. For example, $|\{a, b, c\}| = 3$ and $|\{a, b, a\}| = 2$.[1] Using this notation, we can state the sum principle as: if S_1, S_2, $\ldots S_m$ are disjoint sets, then

$$|S_1 \cup S_2 \cup \cdots \cup S_m| = |S_1| + |S_2| + \cdots + |S_m| \; . \tag{1.2}$$

To write this without the "dots" that indicate left-out material, we write

$$|\bigcup_{i=1}^{m} S_i| = \sum_{i=1}^{m} |S_i|.$$

When we can write a set S as a union of disjoint sets S_1, S_2, $\ldots$, S_k we say that we have *partitioned* S into the sets S_1, S_2, $\ldots$, S_k, and we say that the sets S_1, S_2, $\ldots$, S_k form a *partition* of S. Thus $\{\{1\}, \{3, 5\}, \{2, 4\}\}$ is a partition of the set $\{1, 2, 3, 4, 5\}$ and the set $\{1, 2, 3, 4, 5\}$ can be partitioned into the sets $\{1\}$, $\{3, 5\}$, $\{2, 4\}$. It is clumsy to say we are partitioning a set into sets, so instead we call the sets S_i into which we partition a set S the *blocks* of the partition. Thus the sets $\{1\}$, $\{3, 5\}$, $\{2, 4\}$ are the blocks of a partition of $\{1, 2, 3, 4, 5\}$. In this language, we can restate the sum principle as follows.

Principle 1.2 (Sum Principle) *If a finite set S has been partitioned into blocks, then the size of S is the sum of the sizes of the blocks.*

Abstraction

The process of figuring out a general principle that explains why a certain computation makes sense is an example of the mathematical process of *abstraction*. We won't try to give a precise definition of abstraction but rather point out examples of the process as we proceed. In a course in set theory, we would further abstract our work and derive the sum principle from the axioms of

[1] It may look strange to have $|\{a, b, a\}| = 2$, but an element either is or is not in a set. It cannot be in a set multiple times. (This situation leads to the idea of multisets that will be introduced later on in this section.) We gave this example to emphasize that the notation $\{a, b, a\}$ means the same thing as $\{a, b\}$. Why would someone even contemplate the notation $\{a, b, a\}$. Suppose we wrote $S = \{x | x \text{ is the first letter of Ann, Bob, or Alice}\}$. Explicitly following this description of S would lead us to first write down $\{a, b, a\}$ and the realize it equals $\{a, b\}$.

set theory. In a course in discrete mathematics, this level of abstraction is unnecessary, so we will simply use the sum principle as the basis of computations when it is convenient to do so. If our goal were only to solve this one exercise, then our abstraction would have been almost a mindless exercise that complicated what was an "obvious" solution to Exercise 1.1-1. However the sum principle will prove to be useful in a wide variety of problems. Thus we observe the value of abstraction—when you can recognize the abstract elements of a problem, then abstraction often helps you solve subsequent problems as well.

Summing Consecutive Integers

Returning to the problem in Exercise 1.1-1, it would be nice to find a simpler form for the sum given in Equation 1.1. We may also write this sum as

$$\sum_{i=1}^{n-1} n-i.$$

Now, if we don't like to deal with summing the values of $(n-i)$, we can observe that the values we are summing are $n-1, n-2, \ldots, 1$, so we may write that

$$\sum_{i=1}^{n-1} n-i = \sum_{i=1}^{n-1} i.$$

A clever trick, usually attributed to Gauss, gives us a shorter formula for this sum.

We write

$$\begin{array}{ccccccccccc} & 1 & + & 2 & + & \cdots & + & n-2 & + & n-1 \\ + & n-1 & + & n-2 & + & \cdots & + & 2 & + & 1 \\ \hline & n & + & n & + & \cdots & + & n & + & n \end{array}$$

The sum below the horizontal line has $n-1$ terms each equal to n, and thus it is $n(n-1)$. It is the sum of the two sums above the line, and since these sums are equal (being identical except for being in reverse order), the sum below the line must be twice either sum above, so either of the sums above must be $n(n-1)/2$. In other words, we may write

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

This lovely trick gives us little or no real mathematical skill; learning how to think about things to discover answers ourselves is much more useful. After we analyze Exercise 1.1-2 and abstract the process we are using there, we will be able to come back to this problem at the end of this section and see a way that we could have discovered this formula for ourselves without any tricks.

The Product Principle

Exercise 1.1-2 The loop below is part of a program which computes the product of two matrices. (You don't need to know what the product of two matrices is to answer this question.)

```
(1)  for i = 1 to r
(2)       for j = 1 to m
(3)            S = 0
(4)            for k = 1 to n
(5)                 S = S + A[i,k] * B[k,j]
(6)            C[i,j] = S
```

How many multiplications (expressed in terms of r, m, and n) does this code carry out in line 5?

Exercise 1.1-3 Consider the following longer piece of pseudocode that sorts a list of numbers and then counts "big gaps" in the list (for this problem, a big gap in the list is a place where a number in the list is more than twice the previous number:

```
(1)  for i = 1 to n - 1
(2)       minval = A[i]
(3)       minindex = i
(4)       for j = i to n
(5)            if (A[j] < minval)
(6)                 minval = A[j]
(7)                 minindex = j
(8)       exchange A[i] and A[minindex]
(9)
(10) for i = 2 to n
(11)      if (A[i] > 2 * A[i - 1])
(12)           bigjump = bigjump +1
```

How many comparisons does the above code make in lines 5 and 11 ?

In Exercise 1.1-2, the program segment in lines 4 through 5, which we call the "inner loop," takes exactly n steps, and thus makes n multiplications, regardless of what the variables i and j are. The program segment in lines 2 through 5 repeats the inner loop exactly m times, regardless of what i is. Thus this program segment makes n multiplications m times, so it makes nm multiplications.

Why did we add in Exercise 1.1-1, but multiply here? We can answer this question using the abstract point of view we adopted in discussing Exercise 1.1-1. Our algorithm performs a certain set of multiplications. For any given i, the set of multiplications performed in lines 2 through 5 can be divided into the set S_1 of multiplications performed when $j = 1$, the set S_2 of multiplications performed when $j = 2$, and, in general, the set S_j of multiplications performed for any given j value. Each set S_j consists of those multiplications the inner loop carries out for a particular value of j, and there are exactly n multiplications in this set. Let T_i be the set of multiplications that our program segment carries out for a certain i value. The set T_i is the union of the sets S_j; restating this as an equation, we get

$$T_i = \bigcup_{j=1}^{m} S_j.$$

Then, by the sum principle, the size of the set T_i is the sum of the sizes of the sets S_j, and a sum of m numbers, each equal to n, is mn. Stated as an equation,

$$|T_i| = |\bigcup_{j=1}^{m} S_j| = \sum_{j=1}^{m} |S_j| = \sum_{j=1}^{m} n = mn. \tag{1.3}$$

Thus we are multiplying because multiplication is repeated addition!

From our solution we can extract a second principle that simply shortcuts the use of the sum principle.

Principle 1.3 (Product Principle) *The size of a union of m disjoint sets, each of size n, is mn.*

We now complete our discussion of Exercise 1.1-2. Lines 2 through 5 are executed once for each value of i from 1 to r. Each time those lines are executed, they are executed with a different i value, so the set of multiplications in one execution is disjoint from the set of multiplications in any other execution. Thus the set of all multiplications our program carries out is a union of r disjoint sets T_i of mn multiplications each. Then by the product principle, the set of all multiplications has size rmn, so our program carries out rmn multiplications.

Exercise 1.1-3 demonstrates that thinking about whether the sum or product principle is appropriate for a problem can help to decompose the problem into easily-solvable pieces. If you can decompose the problem into smaller pieces and solve the smaller pieces, then you either add or multiply solutions to solve the larger problem. In this exercise, it is clear that the number of comparisons in the program fragment is the sum of the number of comparisons in the first loop in lines 1 through 8 with the number of comparisons in the second loop in lines 10 through 12 (what two disjoint sets are we talking about here?). Further, the first loop makes $n(n+1)/2 - 1$ comparisons[2], and that the second loop has $n-1$ comparisons, so the fragment makes $n(n+1)/2 - 1 + n - 1 = n(n+1)/2 + n - 2$ comparisons.

Two element subsets

Often, there are several ways to solve a problem. We originally solved Exercise 1.1-1 by using the sum principal, but it is also possible to solve it using the product principal. Solving a problem two ways not only increases our confidence that we have found the correct solution, but it also allows us to make new connections and can yield valuable insight.

Consider the set of comparisons made by the entire execution of the code in this exercise. When $i = 1$, j takes on every value from 2 to n. When $i = 2$, j takes on every value from 3 to n. Thus, for each two numbers i and j, we compare $A[i]$ and $A[j]$ exactly once in our loop. (The order in which we compare them depends on whether i or j is smaller.) Thus the number of comparisons we make is the same as the number of two element subsets of the set $\{1, 2, \ldots, n\}$[3]. In how many ways can we choose two elements from this set? If we choose a first and second element, there are n ways to choose a first element, and for each choice of the first element, there are $n-1$ ways to choose a second element. Thus the set of all such choices is the union of n sets

[2]To see why this is true, ask yourself first where the $n(n+1)/2$ comes from, and then why we subtracted one.

[3]The relationship between the set of comparisons and the set of two-element subsets of $\{1, 2, \ldots, n\}$ is an example of a bijection, an idea which will be examined more in Section 1.2.

of size $n-1$, one set for each first element. Thus it might appear that, by the product principle, there are $n(n-1)$ ways to choose two elements from our set. However, what we have chosen is an *ordered pair*, namely a pair of elements in which one comes first and the other comes second. For example, we could choose 2 first and 5 second to get the ordered pair $(2,5)$, or we could choose 5 first and 2 second to get the ordered pair $(5,2)$. Since each pair of distinct elements of $\{1,2,\ldots,n\}$ can be ordered in two ways, we get twice as many ordered pairs as two element sets. Thus, since the number of ordered pairs is $n(n-1)$, the number of two element subsets of $\{1,2,\ldots,n\}$ is $n(n-1)/2$. Therefore the answer to Exercise 1.1-1 is $n(n-1)/2$. This number comes up so often that it has its own name and notation. We call this number "n choose 2" and denote it by $\binom{n}{2}$. To summarize, $\binom{n}{2}$ stands for the number of two element subsets of an n element set and equals $n(n-1)/2$. Since one answer to Exercise 1.1-1 is $1+2+\cdots+n-1$ and a second answer to Exercise 1.1-1 is $\binom{n}{2}$, this shows that

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

Important Concepts, Formulas, and Theorems

1. *Set.* A *set* is a collection of objects. In a set order is not important. Thus the set $\{A,B,C\}$ is the same as the set $\{A,C,B\}$. An element either is or is not in a set; it cannot be in a set more than once, even if we have a description of a set which names that element more than once.

2. *Disjoint.* Two sets are called *disjoint* when they have no elements in common.

3. *Mutually disjoint sets.* A set of sets $\{S_1,\ldots,S_n\}$ is a family of *mutually disjoint sets*, if each two of the sets S_i are disjoint.

4. *Size of a set.* Given a set S, the size of S, denoted $|S|$, is the number of distinct elements in S.

5. *Sum Principle.* The size of a union of a family of mutually disjoint sets is the sum of the sizes of the sets. In other words, if S_1, S_2, $\ldots S_n$ are disjoint sets, then

   $$|S_1\cup S_2\cup\cdots\cup S_n|=|S_1|+|S_2|+\cdots+|S_n|.$$

   To write this without the "dots" that indicate left-out material, we write

   $$|\bigcup_{i=1}^{n} S_i|=\sum_{i=1}^{n}|S_i|.$$

6. *Partition of a set.* A partition of a set S is a set of mutually disjoint subsets (sometimes called blocks) of S whose union is S.

7. *Sum of first $n-1$ numbers.*

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

8. *Product Principle.* The size of a union of m disjoint sets, each of size n, is mn.

9. *Two element subsets.* $\binom{n}{2}$ stands for the number of two element subsets of an n element set and equals $n(n-1)/2$. $\binom{n}{2}$ is read as "n choose 2."

Problems

1. The segment of code below is part of a program that uses insertion sort to sort a list A

```
for i = 2 to n
    j=i
    while j ≥ 2 and A[j] < A[j − 1]
        exchange A[j] and A[j − 1]
        j − −
```

What is the maximum number of times (considering all lists of n items you could be asked to sort) the program makes the comparison $A[j] < A[j-1]$? Describe as succinctly as you can those lists that require this number of comparisons.

2. Five schools are going to send their baseball teams to a tournament, in which each team must play each other team exactly once. How many games are required?

3. Use notation similar to that in Equations 1.2 and 1.3 to rewrite the solution to Exercise 1.1-3 more algebraically.

4. In how many ways can you draw a first card and then a second card from a deck of 52 cards?

5. In how many ways can you draw two cards from a deck of 52 cards.

6. In how many ways may you draw a first, second, and third card from a deck of 52 cards?

7. In how many ways may a ten person club select a president and a secretary-treasurer from among its members?

8. In how many ways may a ten person club select a two person executive committee from among its members?

9. In how many ways may a ten person club select a president and a two person executive advisory board from among its members (assuming that the president is not on the advisory board)?

10. By using the formula for $\binom{n}{2}$ is is straightforward to show that

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

However this proof just uses blind substitution and simplification. Find a more conceptual explanation of why this formula is true.

11. If M is an m element set and N is an n-element set, how many ordered pairs are there whose first member is in M and whose second member is in N?

12. In the local ice cream shop, there are 10 different flavors. How many different two-scoop cones are there? (Following your mother's rule that it all goes to the same stomach, a cone with a vanilla scoop on top of a chocolate scoop is considered the same as a cone with a a chocolate scoop on top of a vanilla scoop.)

13. Now suppose that you decide to disagree with your mother in Exercise 12 and say that the order of the scoops does matter. How many different possible two-scoop cones are there?

14. Suppose that on day 1 you receive 1 penny, and, for $i > 1$, on day i you receive twice as many pennies as you did on day $i - 1$. How many pennies will you have on day 20? How many will you have on day n? Did you use the sum or product principal?

15. The "Pile High Deli" offers a "simple sandwich" consisting of your choice of one of five different kinds of bread with your choice of butter or mayonnaise or no spread, one of three different kinds of meat, and one of three different kinds of cheese, with the meat and cheese "piled high" on the bread. In how many ways may you choose a simple sandwich?

16. Do you see any unnecessary steps in the pseudocode of Exercise 1.1-3?

1.2 Counting Lists, Permutations, and Subsets.

Using the Sum and Product Principles

Exercise 1.2-1 A password for a certain computer system is supposed to be between 4 and 8 characters long and composed of lower and/or upper case letters. How many passwords are possible? What counting principles did you use? Estimate the percentage of the possible passwords that have exactly four characters.

A good way to attack a counting problem is to ask if we could use either the sum principle or the product principle to simplify or completely solve it. Here that question might lead us to think about the fact that a password can have 4, 5, 6, 7 or 8 characters. The set of all passwords is the union of those with 4, 5, 6, 7, and 8 letters so the sum principle might help us. To write the problem algebraically, let P_i be the set of i-letter passwords and P be the set of all possible passwords. Clearly,

$$P = P_4 \cup P_5 \cup P_6 \cup P_7 \cup P_8 \ .$$

The P_i are mutually disjoint, and thus we can apply the sum principal to obtain

$$|P| = \sum_{i=4}^{8} |P_i| \ .$$

We still need to compute $|P_i|$. For an i-letter password, there are 52 choices for the first letter, 52 choices for the second and so on. Thus by the product principle, $|P_i|$, the number of passwords with i letters is 52^i. Therefore the total number of passwords is

$$52^4 + 52^5 + 52^6 + 52^7 + 52^8.$$

Of these, 52^4 have four letters, so the percentage with 54 letters is

$$\frac{100 \cdot 52^4}{52^4 + 52^5 + 52^6 + 52^7 + 52^8.}$$

Although this is a nasty formula to evaluate by hand, we can get a quite good estimate as follows. Notice that 52^8 is 52 times as big as 52^7, and even more dramatically larger than any other term in the sum in the denominator. Thus the ratio thus just a bit less than

$$\frac{100 \cdot 52^4}{52^8,}$$

which is $100/52^4$, or approximately .000014. Thus to five decimal places, only .00001% of the passwords have four letters. It is therefore much easier guess a password that we know has four letters than it is to guess one that has between 4 and 8 letters—roughly 7 million times easier!

In our solution to Exercise 1.2-1, we casually referred to the use of the product principle in computing the number of passwords with i letters. We didn't write any set as a union of sets of equal size. We could have, but it would have been clumsy and repetitive. For this reason we will state a second version of the product principle that we can derive from the version for unions of sets by using the idea of mathematical induction that we study in Chapter 4.

Version 2 of the *product principle* states:

Principle 1.4 (Product Principle, Version 2) *If a set S of lists of length m has the properties that*

1. *There are i_1 different first elements of lists in S, and*
2. *For each $j > 1$ and each choice of the first $j-1$ elements of a list in S there are i_j choices of elements in position j of those lists,*

then there are $i_1 i_2 \cdots i_m = \prod_{k=1}^{m} i_k$ lists in S.

Let's apply this version of the product principle to compute the number of m-letter passwords. Since an m-letter password is just a list of m letters, and since there are 52 different first elements of the password and 52 choices for each other position of the password, we have that $i_1 = 52,\ i_2 = 52, \ldots, i_m = 52$. Thus, this version of the product principle tells us immediately that the number of passwords of length m is $i_1 i_2 \cdots i_m = 52^m$.

In our statement of version 2 of the Product Principle, we have introduced a new notation, the use of Π to stand for product. This notation is called the *product notation*, and it is used just like summation notation. In particular, $\prod_{k=1}^{m} i_k$ is read as "The product from $k = 1$ to m of i_k." Thus $\prod_{k=1}^{m} i_k$ means the same thing as $i_1 \cdot i_2 \cdots i_m$.

Lists and functions

We have left a term undefined in our discussion of version 2 of the product principle, namely the word "list." A *list* of 3 things chosen from a set T consists of a first member t_1 of T, a second member t_2 of T, and a third member t_3 of T. If we rewrite the list in a different order, we get a different list. A list of k things chosen from T consists of a first member of T through a kth member of T. We can use the word "function," which you probably recall from algebra or calculus, to be more precise.

Recall that a function from a set S (called the *domain* of the function) to a set T (called the *range* of the function) is a relationship between the elements of S and the elements of T that relates exactly one element of T to each element of S. We use a letter like f to stand for a function and use $f(x)$ to stand for the one and only one element of T that the function relates to the element x of S. You are probably used to thinking of functions in terms of formulas like $f(x) = x^2$. We need to use formulas like this in algebra and calculus because the functions that you study in algebra and calculus have infinite sets of numbers as their domains and ranges. In discrete mathematics, functions often have finite sets as their domains and ranges, and so it is possible to describe a function by saying exactly what it is. For example

$$f(1) = \text{Sam},\ f(2) = \text{Mary},\ f(3) = \text{Sarah}$$

is a function that describes a list of three people. This suggests a precise definition of a list of k elements from a set T: A *list of k elements* from a set T is a function from $\{1, 2, \ldots, k\}$ to T.

Exercise 1.2-2 Write down all the functions from the two-element set $\{1, 2\}$ to the two-element set $\{a, b\}$.

Exercise 1.2-3 How many functions are there from a two-element set to a three element set?

Exercise 1.2-4 How many functions are there from a three-element set to a two-element set?

In Exercise 1.2-2 one thing that is difficult is to choose a notation for writing the functions down. We will use f_1, f_2, etc., to stand for the various functions we find. To describe a function f_i from $\{1,2\}$ to $\{a,b\}$ we have to specify $f_i(1)$ and $f_i(2)$. We can write

$$\begin{array}{ll} f_1(1)=a & f_1(2)=b \\ f_2(1)=b & f_2(2)=a \\ f_3(1)=a & f_3(2)=a \\ f_4(1)=b & f_4(2)=b \end{array}$$

We have simply written down the functions as they occurred to us. How do we know we have all of them? The set of all functions from $\{1,2\}$ to $\{a,b\}$ is the union of the functions f_i that have $f_i(1)=a$ and those that have $f_i(1)=b$. The set of functions with $f_i(1)=a$ has two elements, one for each choice of $f_i(2)$. Therefore by the product principle the set of all functions from $\{1,2\}$ to $\{a,b\}$ has size $2\cdot 2=4$.

To compute the number of functions from a two element set (say $\{1,2\}$) to a three element set, we can again think of using f_i to stand for a typical function. Then the set of all functions is the union of three sets, one for each choice of $f_i(1)$. Each of these sets has three elements, one for each choice of $f_i(2)$. Thus by the product principle we have $3\cdot 3=9$ functions from a two element set to a three element set.

To compute the number of functions from a three element set (say $\{1,2,3\}$) to a two element set, we observe that the set of functions is a union of four sets, one for each choice of $f_i(1)$ and $f_i(2)$ (as we saw in our solution to Exercise 1.2-2). But each of these sets has two functions in it, one for each choice of $f_i(3)$. Then by the product principle, we have $4\cdot 2=8$ functions from a three element set to a two element set.

A function f is called *one-to-one* or an *injection* if whenever $x\neq y$, $f(x)\neq f(y)$. Notice that the two functions f_1 and f_2 we gave in our solution of Exercise 1.2-2 are one-to-one, but f_3 and f_4 are not.

A function f is called *onto* or a *surjection* if every element y in the range is $f(x)$ for some x in the domain. Notice that the functions f_1 and f_2 in our solution of Exercise 1.2-2 are onto functions but f_3 and f_4 are not.

Exercise 1.2-5 Using two-element sets or three-element sets as domains and ranges, find an example of a one-to-one function that is not onto.

Exercise 1.2-6 Using two-element sets or three-element sets as domains and ranges, find an example of an onto function that is not one-to-one.

Notice that the function given by $f(1)=c$, $f(2)=a$ is an example of a function from $\{1,2\}$ to $\{a,b,c\}$ that is one-to one but not onto.

Also, notice that the function given by $f(1)=a$, $f(2)=b$, $f(3)=a$ is an example of a function from $\{1,2,3\}$ to $\{a,b\}$ that is onto but not one to one.

The Bijection Principle

Exercise 1.2-7 The loop below is part of a program to determine the number of triangles formed by n points in the plane.

```
(1)  trianglecount = 0
(2)  for i = 1 to n
(3)       for j = i + 1 to n
(4)            for k = j + 1 to n
(5)                 if points i, j, and k are not collinear
(6)                      trianglecount = trianglecount +1
```

How many times does the above code check three points to see if they are collinear in line 5?

In Exercise 1.2-7, we have a loop embedded in a loop that is embedded in another loop. Because the second loop, starting in line 3, begins with $j = i + 1$ and j increase up to n, and because the third loop, starting in line 4, begins with $k = j + 1$ and increases up to n, our code examines each triple of values i, j, k with $i < j < k$ exactly once. For example, if n is 4, then the triples (i, j, k) used by the algorithm, in order, are $(1, 2, 3)$, $(1, 2, 4)$, $(1, 3, 4)$, and $(2, 3, 4)$. Thus one way in which we might have solved Exercise 1.2-7 would be to compute the number of such triples, which we will call *increasing triples*. As with the case of two-element subsets earlier, the number of such triples is the number of three-element subsets of an n-element set. This is the second time that we have proposed counting the elements of one set (in this case the set of increasing triples chosen from an n-element set) by saying that it is equal to the number of elements of some other set (in this case the set of three element subsets of an n-element set). When are we justified in making such an assertion that two sets have the same size? There is another fundamental principle that abstracts our concept of what it means for two sets to have the same size. Intuitively two sets have the same size if we can match up their elements in such a way that each element of one set corresponds to exactly one element of the other set. This description carries with it some of the same words that appeared in the definitions of functions, one-to-one, and onto. Thus it should be no surprise that one-to-one and onto functions are part of our abstract principle.

Principle 1.5 (Bijection Principle) *Two sets have the same size if and only if there is a one-to-one function from one set onto the other.*

Our principle is called the *bijection principle* because a one-to-one and onto function is called a *bijection*. Another name for a bijection is a *one-to-one correspondence*. A bijection from a set to itself is called a *permutation* of that set.

What is the bijection that is behind our assertion that the number of increasing triples equals the number of three-element subsets? We define the function f to be the one that takes the increasing triple (i, j, k) to the subset $\{i, j, k\}$. Since the three elements of an increasing triple are different, the subset is a three element set, so we have a function from increasing triples to three element sets. Two different triples can't be the same set in two different orders, so different triples have to be associated with different sets. Thus f is one-to-one. Each set of three integers can be listed in increasing order, so it is the image under f of an increasing triple. Therefore f is onto. Thus we have a one-to-one correspondence, or bijection, between the set of increasing triples and the set of three element sets.

k-element permutations of a set

Since counting increasing triples is equivalent to counting three-element subsets, we can count increasing triples by counting three-element subsets instead. We use a method similar to the one we used to compute the number of two-element subsets of a set. Recall that the first step was to compute the number of ordered pairs of distinct elements we could chose from the set $\{1, 2, \ldots, n\}$. So we now ask in how many ways may we choose an ordered triple of distinct elements from $\{1, 2, \ldots, n\}$, or more generally, in how many ways may we choose a list of k distinct elements from $\{1, 2, \ldots, n\}$. A list of k-distinct elements chosen from a set N is called a *k-element permutation* of N.[4]

How many 3-element permutations of $\{1, 2, \ldots, n\}$ can we make? Recall that a k-element permutation is a list of k distinct elements. There are n choices for the first number in the list. For each way of choosing the first element, there are $n-1$ choices for the second. For each choice of the first two elements, there are $n-2$ ways to choose a third (distinct) number, so by version 2 of the product principle, there are $n(n-1)(n-2)$ ways to choose the list of numbers. For example, if n is 4, the three-element permutations of $\{1, 2, 3, 4\}$ are

$$\begin{aligned} L \;=\; & \{123, 124, 132, 134, 142, 143, 213, 214, 231, 234, 241, 243, \\ & 312, 314, 321, 324, 341, 342, 412, 413, 421, 423, 431, 432\}. \end{aligned} \tag{1.4}$$

There are indeed $4 \cdot 3 \cdot 2 = 24$ lists in this set. Notice that we have listed the lists in the order that they would appear in a dictionary (assuming we treated numbers as we treat letters). This ordering of lists is called the *lexicographic ordering*.

A general pattern is emerging. To compute the number of k-element permutations of the set $\{1, 2, \ldots, n\}$, we recall that they are lists and note that we have n choices for the first element of the list, and regardless of which choice we make, we have $n-1$ choices for the second element of the list, and more generally, given the first $i-1$ elements of a list we have $n-(i-1) = n-i+1$ choices for the ith element of the list. Thus by version 2 of the product principle, we have $n(n-1)\cdots(n-k+1)$ (which is the first k terms of $n!$) ways to choose a k-element permutation of $\{1, 2, \ldots, n\}$. There is a very handy notation for this product first suggested by Don Knuth. We use $n^{\underline{k}}$ to stand for $n(n-1)\cdots(n-k+1) = \prod_{i=0}^{k-1} n-i$, and call it the *$k$th falling factorial power of n*. We can summarize our observations in a theorem.

Theorem 1.1 *The number k-element permutations of an n-element set is*

$$n^{\underline{k}} = \prod_{i=0}^{k-1} n-i = n(n-1)\cdots(n-k+1) = n!/(n-k)!\ .$$

Counting subsets of a set

We now return to the question of counting the number of three element subsets of a $\{1, 2, \ldots, n\}$. We use $\binom{n}{3}$, which we read as "n choose 3" to stand for the number of three element subsets of

[4] In particular a k-element permutation of $\{1, 2, \ldots k\}$ is a list of k distinct elements of $\{1, 2, \ldots, k\}$, which, by our definition of a list is a function from $\{1, 2, \ldots, k\}$ to $\{1, 2, \ldots, k\}$. This function must be one-to-one since the elements of the list are distinct. Since there are k distinct elements of the list, every element of $\{1, 2, \ldots, k\}$ appears in the list, so the function is onto. Therefore it is a bijection. Thus our definition of a permutation of a set is consistent with our definition of a k-element permutation in the case where the set is $\{1, 2, \ldots, k\}$.

$\{1, 2, \ldots, n\}$, or more generally of any n-element set. We have just carried out the first step of computing $\binom{n}{3}$ by counting the number of three-element permutations of $\{1, 2, \ldots, n\}$.

Exercise 1.2-8 Let L be the set of all three-element permutations of $\{1, 2, 3, 4\}$, as in Equation 1.4. How many of the lists (permutations) in L are lists of the 3 element set $\{1, 3, 4\}$? What are these lists?

We see that this set appears in L as 6 different lists: 134, 143, 314, 341, 413, and 431. In general given three different numbers with which to create a list, there are three ways to choose the first number in the list, given the first there are two ways to choose the second, and given the first two there is only one way to choose the third element of the list. Thus by version 2 of the product principle once again, there are $3 \cdot 2 \cdot 1 = 6$ ways to make the list.

Since there are $n(n-1)(n-2)$ permutations of an n-element set, and each three-element subset appears in exactly 6 of these lists, the number of three-element permutations is six times the number of three element subsets. That is, $n(n-1)(n-2) = \binom{n}{3} \cdot 6$. Whenever we see that one number that counts something is the product of two other numbers that count something, we should expect that there is an argument using the product principle that explains why. Thus we should be able to see how to break the set of all 3-element permutations of $\{1, 2, \ldots, n\}$ into either 6 disjoint sets of size $\binom{n}{3}$ or into $\binom{n}{3}$ subsets of size six. Since we argued that each three element subset corresponds to six lists, we have described how to get a set of six lists from one three-element set. Two different subsets could never give us the same lists, so our sets of three-element lists are disjoint. In other words, we have divided the set of all three-element permutations into $\binom{n}{3}$ mutually sets of size six. In this way the product principle does explain why $n(n-1)(n-2) = \binom{n}{3} \cdot 6$. By division we get that we have

$$\binom{n}{3} = n(n-1)(n-2)/6$$

three-element subsets of $\{1, 2, \ldots, n\}$. For $n = 4$, the number is $4(3)(2)/6 = 4$. These sets are $\{1, 2, 3\}$, $\{1, 2, 4\}$, $\{1, 3, 4\}$, and $\{2, 3, 4\}$. It is straightforward to verify that each of these sets appears 6 times in L, as 6 different lists.

Essentially the same argument gives us the number of k-element subsets of $\{1, 2, \ldots, n\}$. We denote this number by $\binom{n}{k}$, and read it as "n choose k." Here is the argument: the set of all k-element permutations of $\{1, 2, \ldots, n\}$ can be partitioned into $\binom{n}{k}$ disjoint blocks[5], each block consisting of all k-element permutations of a k-element subset of $\{1, 2, \ldots, n\}$. But the number of k-element permutations of a k-element set is $k!$, either by version 2 of the product principle or by Theorem 1.1. Thus by version 1 of the product principle we get the equation

$$n^{\underline{k}} = \binom{n}{k} k!.$$

Division by $k!$ gives us our next theorem.

Theorem 1.2 *For integers n and k with $0 \leq k \leq n$, the number of k element subsets of an n element set is*

$$\frac{n^{\underline{k}}}{k!} = \frac{n!}{k!(n-k)!}$$

[5]Here we are using the language introduced for partitions of sets in Section 1.1

Proof: The proof is given above, except in the case that k is 0; however the only subset of our n-element set of size zero is the empty set, so we have exactly one such subset. This is exactly what the formula gives us as well. (Note that the cases $k = 0$ and $k = n$ both use the fact that $0! = 1$.[6]) The equality in the theorem comes from the definition of $n^{\underline{k}}$. ■

Another notation for the numbers $\binom{n}{k}$ is $C(n,k)$. Thus we have that

$$C(n,k) = \binom{n}{k} = \frac{n!}{k!(n-k)!}. \tag{1.5}$$

These numbers are called *binomial coefficients* for reasons that will become clear later.

Important Concepts, Formulas, and Theorems

1. *List.* A list of k items chosen from a set X is a function from $\{1, 2, \ldots k\}$ to X.

2. *Lists versus sets.* In a list, the order in which elements appear in the list matters, and an element may appear more than once. In a set, the order in which we write down the elements of the set does not matter, and an element can appear at most once.

3. *Product Principle, Version 2.* If a set S of lists of length m has the properties that

   (a) There are i_1 different first elements of lists in S, and

   (b) For each $j > 1$ and each choice of the first $j-1$ elements of a list in S there are i_j choices of elements in position j of those lists,

   then there are $i_1 i_2 \cdots i_m$ lists in S.

4. *Product Notaton.* We use the Greek letter Π to stand for product just as we use the Greek letter Σ to stand for sum. This notation is called the *product notation*, and it is used just like summation notation. In particular, $\prod_{k=1}^{m} i_k$ is read as "The product from $k = 1$ to m of i_k." Thus $\prod_{k=1}^{m} i_k$ means the same thing as $i_1 \cdot i_2 \cdots i_m$.

5. *Function.* A *function* f from a set S to a set T is a relationship between S and T that relates exactly one element of T to each element of S. We write $f(x)$ for the one and only one element of T that the function f relates to the element x of S. The same element of T may be related to different members of S.

6. *Onto, Surjection* A function f from a set S to a set T is *onto* if for each element $y \in T$, there is at least one $x \in S$ such that $f(x) = y$. An onto function is also called a *surjection.*

7. *One-to-one, Injection.* A function f from a set S to a set T is *one-to-one* if, for each $x \in S$ and $y \in S$ with $x \neq y$, $f(x) \neq f(y)$. A one-to-one function is also called an *injection.*

8. *Bijection, One-to-one correspondence.* A function from a set S to a set T is a *bijection* if it is both one-to-one and onto. A bijection is sometimes called a *one-to-one correspondence.*

9. *Permutation.* A one-to-one function from a set S to S is called a *permutation* of S.

[6]There are many reasons why 0! is defined to be one; making the formula for $\binom{n}{k}$ work out is one of them.

10. *k-element permutation.* A *k-element permutation* of a set S is a list of k distinct elements of S.

11. *k-element subsets. n choose k. Binomial Coefficients.* For integers n and k with $0 \le k \le n$, the number of k element subsets of an n element set is $n!/k!(n-k)!$. The number of k-element subsets of an n-element set is usually denoted by $\binom{n}{k}$ or $C(n,k)$, both of which are read as "n choose k." These numbers are called *binomial coefficients*.

12. The number of k-element permutations of an n-element set is

$$n^{\underline{k}} = n(n-1)\cdots(n-k+1) = n!/(n-k)!.$$

13. When we have a formula to count something and the formula expresses the result as a product, it is useful to try to understand whether and how we could use the product principle to prove the formula.

Problems

1. The "Pile High Deli" offers a "simple sandwich" consisting of your choice of one of five different kinds of bread with your choice of butter or mayonnaise or no spread, one of three different kinds of meat, and one of three different kinds of cheese, with the meat and cheese "piled high" on the bread. In how many ways may you choose a simple sandwich?

2. In how many ways can we pass out k distinct pieces of fruit to n children (with no restriction on how many pieces of fruit a child may get)?

3. Write down all the functions from the three-element set $\{1,2,3\}$ to the set $\{a,b\}$. Indicate which functions, if any, are one-to-one. Indicate which functions, if any, are onto.

4. Write down all the functions form the two element set $\{1,2\}$ to the three element set $\{a,b,c\}$ Indicate which functions, if any, are one-to-one. Indicate which functions, if any, are onto.

5. There are more functions from the real numbers to the real numbers than most of us can imagine. However in discrete mathematics we often work with functions from a finite set S with s elements to a finite set T with t elements. Then there are only a finite number of functions from S to T. How many functions are there from S to T in this case?

6. Assuming $k \le n$, in how many ways can we pass out k distinct pieces of fruit to n children if each child may get at most one? What is the number if $k > n$? Assume for both questions that we pass out all the fruit.

7. Assume $k \le n$, in how many ways can we pass out k identical pieces of fruit to n children if each child may get at most one? What is the number if $k > n$? Assume for both questions that we pass out all the fruit.

8. What is the number of five digit (base ten) numbers? What is the number of five digit numbers that have no two consecutive digits equal? What is the number that have at least one pair of consecutive digits equal?

9. We are making a list of participants in a panel discussion on allowing alcohol on campus. They will be sitting behind a table in the order in which we list them. There will be four administrators and four students. In how many ways may we list them if the administrators must sit together in a group and the students must sit together in a group? In how many ways may we list them if we must alternate students and administrators?

10. (This problem is for students who are working on the relationship between k-element permutations and k-element subsets.) Write down all three element permutations of the five element set $\{1, 2, 3, 4, 5\}$ in lexicographic order. Underline those that correspond to the set $\{1, 3, 5\}$. Draw a rectangle around those that correspond to the set $\{2, 4, 5\}$. How many three-element permutations of $\{1, 2, 3, 4, 5\}$ correspond to a given 3-element set? How many three-element subsets does the set $\{1, 2, 3, 4, 5\}$ have?

11. In how many ways may a class of twenty students choose a group of three students from among themselves to go to the professor and explain that the three-hour labs are actually taking ten hours?

12. We are choosing participants for a panel discussion allowing on allowing alcohol on campus. We have to choose four administrators from a group of ten administrators and four students from a group of twenty students. In how many ways may we do this?

13. We are making a list of participants in a panel discussion on allowing alcohol on campus. They will be sitting behind a table in the order in which we list them. There will be four administrators chosen from a group of ten administrators and four students chosen from a group of twenty students. In how many ways may we choose and list them if the administrators must sit together in a group and the students must sit together in a group? In how many ways may we choose and list them if we must alternate students and administrators?

14. In the local ice cream shop, you may get a sundae with two scoops of ice cream from 10 flavors (in accordance with your mother's rules from Problem 12 in Section 1.1, the way the scoops sit in the dish does not matter), any one of three flavors of topping, and any (or all or none) of whipped cream, nuts and a cherry. How many different sundaes are possible?

15. In the local ice cream shop, you may get a three-way sundae with three of the ten flavors of ice cream, any one of three flavors of topping, and any (or all or none) of whipped cream, nuts and a cherry. How many different sundaes are possible(in accordance with your mother's rules from Problem 12 in Section 1.1, the way the scoops sit in the dish does not matter) ?

16. A tennis club has $2n$ members. We want to pair up the members by twos for singles matches. In how many ways may we pair up all the members of the club? Suppose that in addition to specifying who plays whom, for each pairing we say who serves first. Now in how many ways may we specify our pairs?

17. A basketball team has 12 players. However, only five players play at any given time during a game. In how may ways may the coach choose the five players? To be more realistic, the five players playing a game normally consist of two guards, two forwards, and one center. If there are five guards, four forwards, and three centers on the team, in how many ways can the coach choose two guards, two forwards, and one center? What if one of the centers is equally skilled at playing forward?

18. Explain why a function from an n-element set to an n-element set is one-to-one if and only if it is onto.

19. The function g is called an *inverse* to the function f if the domain of g is the range of f, if $g(f(x)) = x$ for every x in the domain of f and if $f(g(y)) = y$ for each y in the range of f.

    (a) Explain why a function is a bijection if and only if it has an inverse function.

    (b) Explain why a function that has an inverse function has only one inverse function.

1.3 Binomial Coefficients

In this section, we will explore various properties of binomial coefficients. Remember that we defined the quantitu $\binom{m}{k}$ to be the number of k-element subsets of an n-element set.

Pascal's Triangle

Table 1 contains the values of the binomial coefficients $\binom{n}{k}$ for $n = 0$ to 6 and all relevant k values. The table begins with a 1 for $n = 0$ and $k = 0$, because the empty set, the set with no elements, has exactly one 0-element subset, namely itself. We have not put any value into the table for a value of k larger than n, because we haven't directly said what we mean by the binomial coefficient $\binom{n}{k}$ in that case. However, since there are no subsets of an n-element set that have size larger than n, it is natural to say that $\binom{n}{k}$ is zero when $k > n$. Therefore we define $\binom{n}{k}$ to be zero[7] when $k > n$. Thus we could could fill in the empty places in the table with zeros. The table is easier to read if we don't fill in the empty spaces, so we just remember that they are zero.

Table 1.1: A table of binomial coefficients

$n\backslash k$	0	1	2	3	4	5	6
0	1						
1	1	1					
2	1	2	1				
3	1	3	3	1			
4	1	4	6	4	1		
5	1	5	10	10	5	1	
6	1	6	15	20	15	6	1

Exercise 1.3-1 What general properties of binomial coefficients do you see in Table 1.1

Exercise 1.3-2 What is the next row of the table of binomial coefficients?

Several properties of binomial coefficients are apparent in Table 1.1. Each row begins with a 1, because $\binom{n}{0}$ is always 1. This is the case because there is just one subset of an n-element set with 0 elements, namely the empty set. Similarly, each row ends with a 1, because an n-element set S has just one n-element subset, namely S itself. Each row increases at first, and then decreases. Further the second half of each row is the reverse of the first half. The array of numbers called *Pascal's Triangle* emphasizes that symmetry by rearranging the rows of the table so that they line up at their centers. We show this array in Table 2. When we write down Pascal's triangle, we leave out the values of n and k.

You may know a method for creating Pascal's triangle that does not involve computing binomial coefficients, but rather creates each row from the row above. Each entry in Table 1.2, except for the ones, is the sum of the entry directly above it to the left and the entry directly

[7] If you are thinking "But we did define $\binom{n}{k}$ to be zero when $k > n$ by saying that it is the number of k element subsets of an n-element set, so of course it is zero," then good for you.

Table 1.2: Pascal's Triangle

						1						
					1		1					
				1		2		1				
			1		3		3		1			
		1		4		6		4		1		
	1		5		10		10		5		1	
1		6		15		20		15		6		1

above it to the right. We call this the *Pascal Relationship*, and it gives another way to compute binomial coefficients without doing the multiplying and dividing in Equation 1.5. If we wish to compute many binomial coefficients, the Pascal relationship often yields a more efficient way to do so. Once the coefficients in a row have been computed, the coefficients in the next row can be computed using only one addition per entry.

We now verify that the two methods for computing Pascal's triangle always yield the same result. In order to do so, we need an algebraic statement of the Pascal Relationship. In Table 1.1, each entry is the sum of the one above it and the one above it and to the left. In algebraic terms, then, the Pascal Relationship says

$$\binom{n}{k} = \binom{n-1}{k-1} + \binom{n-1}{k}, \tag{1.6}$$

whenever $n > 0$ and $0 < k < n$. It is possible to give a purely algebraic (and rather dreary) proof of this formula by plugging in our earlier formula for binomial coefficients into all three terms and verifying that we get an equality. A guiding principle of discrete mathematics is that when we have a formula that relates the numbers of elements of several sets, we should find an explanation that involves a relationship among the sets.

A proof using the Sum Principle

From Theorem 1.2 and Equation 1.5, we know that the expression $\binom{n}{k}$ is the number of k-element subsets of an n element set. Each of the three terms in Equation 1.6 therefore represents the number of subsets of a particular size chosen from an appropriately sized set. In particular, the three terms are the number of k-element subsets of an n-element set, the number of $(k-1)$-element subsets of an $(n-1)$-element set, and the number of k-element subsets of an $(n-1)$-element set. We should, therefore, be able to explain the relationship among these three quantities using the sum principle. This explanation will provide a proof, just as valid a proof as an algebraic derivation. Often, a proof using the sum principle will be less tedious, and will yield more insight into the problem at hand.

Before giving such a proof in Theorem 1.3 below, we work out a special case. Suppose $n = 5$, $k = 2$. Equation 1.6 says that

$$\binom{5}{2} = \binom{4}{1} + \binom{4}{2}. \tag{1.7}$$

Because the numbers are small, it is simple to verify this by using the formula for binomial coefficients, but let us instead consider subsets of a 5-element set. Equation 1.7 says that the number of 2 element subsets of a 5 element set is equal to the number of 1 element subsets of a 4 element set plus the number of 2 element subsets of a 4 element set. But to apply the sum principle, we would need to say something stronger. To apply the sum principle, we should be able to partition the set of 2 element subsets of a 5 element set into 2 disjoint sets, one of which has the same size as the number of 1 element subsets of a 4 element set and one of which has the same size as the number of 2 element subsets of a 4 element set. Such a partition provides a proof of Equation 1.7. Consider now the set $S = \{A, B, C, D, E\}$. The set of two element subsets is

$$S_1 = \{\{A, B\}, \{AC\}, \{A, D\}, \{A, E\}, \{B, C\}, \{B, D\}, \{B, E\}, \{C, D\}, \{C, E\}, \{D, E\}\}.$$

We now partition S_1 into 2 blocks, S_2 and S_3. S_2 contains all sets in S_1 that do contain the element E, while S_3 contains all sets in S_1 that do not contain the element E. Thus,

$$S_2 = \{\{AE\}, \{BE\}, \{CE\}, \{DE\}\}$$

and

$$S_3 = \{\{AB\}, \{AC\}, \{AD\}, \{BC\}, \{BD\}, \{CD\}\}.$$

Each set in S_2 must contain E and thus contains one other element from S. Since there are 4 other elements in S that we can choose along with E, we have $|S_2| = \binom{4}{1}$. Each set in S_3 contains 2 elements from the set $\{A, B, C, D\}$. There are $\binom{4}{2}$ ways to choose such a two-element subset of $\{A < B < C < D\}$. But $S_1 = S_2 \cup S_3$ and S_2 and S_3 are disjoint, and so, by the sum principle, Equation 1.7 must hold.

We now give a proof for general n and k.

Theorem 1.3 *If n and k are integers with $n > 0$ and $0 < k < n$, then*

$$\binom{n}{k} = \binom{n-1}{k-1} + \binom{n-1}{k}.$$

Proof: The formula says that the number of k-element subsets of an n-element set is the sum of two numbers. As in our example, we will apply the sum principle. To apply it, we need to represent the set of k-element subsets of an n-element set as a union of two other disjoint sets. Suppose our n-element set is $S = \{x_1, x_2, \dots x_n\}$. Then we wish to take S_1, say, to be the $\binom{n}{k}$-element set of all k-element subsets of S and partition it into two disjoint sets of k-element subsets, S_2 and S_3, where the sizes of S_2 and S_3 are $\binom{n-1}{k-1}$ and $\binom{n-1}{k}$ respectively. We can do this as follows. Note that $\binom{n-1}{k}$ stands for the number of k element subsets of the first $n-1$ elements $x_1, x_2, \dots, x_{n-1}$ of S. Thus we can let S_3 be the set of k-element subsets of S that don't contain x_n. Then the only possibility for S_2 is the set of k-element subsets of S that *do* contain x_n. How can we see that the number of elements of this set S_2 is $\binom{n-1}{k-1}$? By observing that removing x_n from each of the elements of S_2 gives a $(k-1)$-element subset of $S' = \{x_1, x_2, \dots x_{n-1}\}$. Further each $(k-1)$-element subset of S' arises in this way from one and only one k-element subset of S containing x_n. Thus the number of elements of S_2 is the number of $(k-1)$-element subsets of S', which is $\binom{n-1}{k-1}$. Since S_2 and S_3 are two disjoint sets whose union is S, the sum principle shows that the number of elements of S is $\binom{n-1}{k-1} + \binom{n-1}{k}$. ■

Notice that in our proof, we used a bijection that we did not explicitly describe. Namely, there is a bijection f between S_3 (the k-element sets of S that contain x_n) and the $(k-1)$-element subsets of S'. For any subset K in S_3, We let $f(K)$ be the set we obtain by removing x_n from K. It is immediate that this is a bijection, and so the bijection principle tells us that the size of S_3 is the size of the set of all subsets of S'.

The Binomial Theorem

Exercise 1.3-3 What is $(x+y)^3$? What is $(x+1)^4$? What is $(2+y)^4$? What is $(x+y)^4$?

The number of k-element subsets of an n-element set is called a *binomial coefficient* because of the role that these numbers play in the algebraic expansion of a binomial $x+y$. The **Binomial Theorem** states that

Theorem 1.4 (Binomial Theorem) *For any integer $n \geq 0$*

$$(x+y)^n = \binom{n}{0}x^n + \binom{n}{1}x^{n-1}y + \binom{n}{2}x^{n-2}y^2 + \cdots + \binom{n}{n-1}xy^{n-1} + \binom{n}{n}y^n, \tag{1.8}$$

or in summation notation,

$$(x+y)^n = \sum_{i=0}^{n} \binom{n}{i} x^{n-i}y^i \ .$$

Unfortunately when most people first see this theorem, they do not have the tools to see easily why it is true. Armed with our new methodology of using subsets to prove algebraic identities, we can give a proof of this theorem.

Let us begin by considering the example $(x+y)^3$ which by the binomial theorem is

$$\begin{aligned} (x+y)^3 &= \binom{3}{0}x^3 + \binom{3}{1}x^2y + \binom{3}{2}xy^2 + \binom{3}{3}y^3 & (1.9) \\ &= x^3 + 3x^2y + 3xy^2 + x^3 \ . & (1.10) \end{aligned}$$

Suppose that we did not know the binomial theorem but still wanted to compute $(x+y)^3$. Then we would write out $(x+y)(x+y)(x+y)$ and perform the multiplication. Probably we would multiply the first two terms, obtaining $x^2 + 2xy + y^2$, and then multiply this expression by $x+y$. Notice that by applying distributive laws you get

$$(x+y)(x+y) = (x+y)x + (x+y)y = xx + xy + yx + y. \tag{1.11}$$

We could use the commutative law to put this into the usual form, but let us hold off for a moment so we can see a pattern evolve. To compute $(x+y)^3$, we can multiply the expression on the right hand side of Equation 1.11 by $x+y$ using the distributive laws to get

$$\begin{aligned} (xx+xy+yx+yy)(x+y) &= (xx+xy+yx+yy)x + (xx+xy+yx+yy)y & (1.12) \\ &= xxx + xyx + yxx + yxx + xxy + xyy + yxy + yyy & (1.13) \end{aligned}$$

Each of these 8 terms that we got from the distributive law may be thought of as a product of terms, one from the first binomial, one from the second binomial, and one from the third binomial. Multiplication is commutative, so many of these products are the same. In fact, we have one xxx or x^3 product, three products with two x's and one y, or x^2y, three products with one x and two y's, or xy^2 and one product which becomes y^3. Now look at Equation 1.9, which summarizes this process. There are $\binom{3}{0} = 1$ way to choose a product with 3 x's and 0 y's, $\binom{3}{1} = 3$ way to choose a product with 2 x's and 1 y, etc. Thus we can understand the binomial theorem as counting the subsets of our binomial factors from which we choose a y-term to get a product with k y's in multiplying a string of n binomials.

Essentially the same explanation gives us a proof of the binomial theorem. Note that when we multiplied out three factors of $(x+y)$ using the distributive law but not collecting like terms, we had a sum of eight products. Each factor of $(x+y)$ doubles the number of summands. Thus when we apply the distributive law as many times as possible (without applying the commutative law and collecting like terms) to a product of n binomials all equal to (x+y), we get 2^n summands. Each summand is a product of a length n list of x's and y's. In each list, the ith entry comes from the ith binomial factor. A list that becomes $x^{n-k}y^k$ when we use the commutative law will have a y in k of its places and an x in the remaining places. The number of lists that have a y in k places is thus the number of ways to select k binomial factors to contribute a y to our list. But the number of ways to select k binomial factors from n binomial factors is simply $\binom{n}{k}$, and so that is the coefficient of $x^{n-k}y^k$. This proves the binomial theorem.

Applying the Binomial Theorem to the remaining questions in Exercise 1.3-3 gives us

$$\begin{aligned}
(x+1)^4 &= x^4 + 4x^3 + 6x^2 + 4x + 1 \\
(2+y)^4 &= 16 + 32y + 24y^2 + 8y^3 + y^4 \text{ and} \\
(x+y)^4 &= x^4 + 4x^3y + 6x^2y^2 + 4xy^3 + y^4.
\end{aligned}$$

Labeling and trinomial coefficients

Exercise 1.3-4 Suppose that I have k labels of one kind and $n-k$ labels of another. In how many different ways may I apply these labels to n objects?

Exercise 1.3-5 Show that if we have k_1 labels of one kind, k_2 labels of a second kind, and $k_3 = n - k_1 - k_2$ labels of a third kind, then there are $\frac{n!}{k_1!k_2!k_3!}$ ways to apply these labels to n objects.

Exercise 1.3-6 What is the coefficient of $x^{k_1}y^{k_2}z^{k_3}$ in $(x+y+z)^n$?

Exercise 1.3-4 and Exercise 1.3-5 can be thought of as immediate applications of binomial coefficients. For Exercise 1.3-4, there are $\binom{n}{k}$ ways to choose the k objects that get the first label, and the other objects get the second label, so the answer is $\binom{n}{k}$. For Exercise 1.3-5, there are $\binom{n}{k_1}$ ways to choose the k_1 objects that get the first kind of label, and then there are $\binom{n-k_1}{k_2}$ ways to choose the objects that get the second kind of label. After that, the remaining $k_3 = n - k_1 - k_2$ objects get the third kind of label. The total number of labellings is thus, by the product principle, the product of the two binomial coefficients, which simplifies as follows.

$$\binom{n}{k_1}\binom{n-k_1}{k_2} = \frac{n!}{k_1!(n-k_1)!}\frac{(n-k_1)!}{k_2!(n-k_1-k_2)!}$$

$$= \frac{n!}{k_1!k_2!(n-k_1-k_2)!}$$
$$= \frac{n!}{k_1!k_2!k_3!}\ .$$

A more elegant approach to Exercise 1.3-4, Exercise 1.3-5, and other related problems appears in the next section.

Exercise 1.3-6 shows how Exercise 1.3-5 applies to computing powers of trinomials. In expanding $(x+y+z)^n$, we think of writing down n copies of the trinomial $x+y+z$ side by side, and applying the distributive laws until we have a sum of terms each of which is a product of x's, y's and z's. How many such terms do we have with k_1 x's, k_2 y's and k_3 z's? Imagine choosing x from some number k_1 of the copies of the trinomial, choosing y from some number k_2, and z from the remaining k_3 copies, multiplying all the chosen terms together, and adding up over all ways of picking the k_is and making our choices. Choosing x from a copy of the trinomial "labels" that copy with x, and the same for y and z, so the number of choices that yield $x^{k_1}y^{k_2}z^{k_3}$ is the number of ways to label n objects with k_1 labels of one kind, k_2 labels of a second kind, and k_3 labels of a third. Notice that this requires that $k_3 = n - k_1 - k_2$. By analogy with our notation for a binomial coefficient, we define the *trinomial coefficient* $\binom{n}{k_1,k_2,k_3}$ to be $\frac{n!}{k_1!k_2!k_3!}$ if $k_1+k_2+k_3 = n$ and 0 otherwise. Then $\binom{n}{k_1,k_2,k_3}$ is the coefficient of $x^{k_1}y^{k_2}z^{k_3}$in $(x+y+z)^n$. This is sometimes called the *trinomial theorem.*

Important Concepts, Formulas, and Theorems

1. *Pascal Relationship.* The Pascal Relationship says that
$$\binom{n}{k} = \binom{n-1}{k-1} + \binom{n-1}{k}\ ,$$
whenever $n > 0$ and $0 < k < n$.

2. *Pascal's Triangle.* Pascal's Triangle is the triangular array of numbers we get by putting ones in row n and column 0 and in row n and column n of a table for every positive integer n and then filling the remainder of the table by letting the number in row n and column j be the sum of the numbers in row $n-1$ and columns $j-1$ and j whenever $0 < j < n$.

3. *Binomial Theorem.* The **Binomial Theorem** states that for any integer $n \geq 0$
$$(x+y)^n = x^n + \binom{n}{1}x^{n-1}y + \binom{n}{2}x^{n-2}y^2 + \cdots + \binom{n}{n-1}xy^{n-1} + \binom{n}{n}y^n\ ,$$
or in summation notation,
$$(x+y)^n = \sum_{i=0}^{n}\binom{n}{i}x^{n-i}y^i\ .$$

4. *Labeling.* The number of ways to apply k labels of one kind and $n-k$ labels of another kind to n objects is $\binom{n}{k}$.

5. *Trinomial coefficient.* We define the *trinomial coefficient* $\binom{n}{k_1,k_2,k_3}$ to be $\frac{n!}{k_1!k_2!k_3!}$ if $k_1+k_2+k_3 = n$ and 0 otherwise.

6. *Trinomial Theorem.* The coefficient of $x^iy^jz^k$ in $(x+y+z)^n$ is $\binom{n}{i,j,k}$.

Problems

1. Find $\binom{12}{3}$ and $\binom{12}{9}$. What can you say in general about $\binom{n}{k}$ and $\binom{n}{n-k}$?

2. Find the row of the Pascal triangle that corresponds to $n = 8$.

3. Find the following

   a. $(x+1)^5$
   b. $(x+y)^5$
   c. $(x+2)^5$
   d. $(x-1)^5$

4. Carefully explain the proof of the binomial theorem for $(x+y)^4$. That is, explain what each of the binomial coefficients in the theorem stands for and what powers of x and y are associated with them in this case.

5. If I have ten distinct chairs to paint, in how many ways may I paint three of them green, three of them blue, and four of them red? What does this have to do with labellings?

6. When n_1, n_2, $\ldots n_k$ are nonnegative integers that add to n, the number $\frac{n!}{n_1!, n_2!, \ldots, n_k!}$ is called a *multinomial coefficient* and is denoted by $\binom{n}{n_1, n_2, \ldots, n_k}$. A polynomial of the form $x_1 + x_2 + \cdots + x_k$ is called a multinomial. Explain the relationship between powers of a multinomial and multinomial coefficients. This relationship is called the Multinomial Theorem.

7. Give a bijection that proves your statement about $\binom{n}{k}$ and $\binom{n}{n-k}$ in Problem 1 of this section.

8. In a Cartesian coordinate system, how many paths are there from the origin to the point with integer coordinates (m, n) if the paths are built up of exactly $m + n$ horizontal and vertical line segments each of length one?

9. What is the formula we get for the binomial theorem if, instead of analyzing the number of ways to choose k distinct y's, we analyze the number of ways to choose k distinct x's?

10. Explain the difference between choosing four disjoint three element sets from a twelve element set and labelling a twelve element set with three labels of type 1, three labels of type two, three labels of type 3, and three labels of type 4. What is the number of ways of choosing three disjoint four element subsets from a twelve element set? What is the number of ways of choosing four disjoint three element subsets from a twelve element set?

11. A 20 member club must have a President, Vice President, Secretary and Treasurer as well as a three person nominations committee. If the officers must be different people, and if no officer may be on the nominating committee, in how many ways could the officers and nominating committee be chosen? Answer the same question if officers may be on the nominating committee.

12. Prove Equation 1.6 by plugging in the formula for $\binom{n}{k}$.

13. Give two proofs that
$$\binom{n}{k} = \binom{n}{n-k}.$$

14. Give at least two proofs that
$$\binom{n}{k}\binom{k}{j} = \binom{n}{j}\binom{n-j}{k-j}.$$

15. Give at least two proofs that
$$\binom{n}{k}\binom{n-k}{j} = \binom{n}{j}\binom{n-j}{k}.$$

16. You need not compute all of rows 7, 8, and 9 of Pascal's triangle to use it to compute $\binom{9}{6}$. Figure out which entries of Pascal's triangle not given in Table 2 you actually need, and compute them to get $\binom{9}{6}$.

17. Explain why
$$\sum_{i=0}^{n}(-1)^i\binom{n}{i} = 0$$

18. Apply calculus and the binomial theorem to $(1+x)^n$ to show that
$$\binom{n}{1} + 2\binom{n}{2} + 3\binom{n}{3} + \cdots = n2^{n-1}.$$

19. True or False: $\binom{n}{k} = \binom{n-2}{k-2} + \binom{n-2}{k-1} + \binom{n-2}{k}$. If true, give a proof. If false, give a value of n and k that show the statement is false, find an analogous true statement, and prove it.

1.4 Equivalence Relations and Counting (Optional)

The Symmetry Principle

Consider again the example from Section 1.2 in which we wanted to count the number of 3 element subsets of a four element set. To do so, we first formed all possible lists of $k = 3$ distinct elements chosen from an $n = 4$ element set. (See Equation 1.4.) The number of lists of k distinct elements is $n^{\underline{k}} = n!/(n-k)!$. We then observed that two lists are equivalent as sets, if one can be obtained by rearranging (or "permuting") the other. This process divides the lists up into classes, called *equivalence classes*, each of size $k!$. Returning to our example in Section 1.2, we noted that one such equivalence class was

$$\{134, 143, 314, 341, 413, 431\}.$$

The other three are

$$\{234, 243, 324, 342, 423, 432\},$$

$$\{132, 123, 312, 321, 213, 231\},$$

and

$$\{124, 142, 214, 241, 412, 421\}.$$

The product principle told us that if q is the number of such equivalence class, if each equivalence class has $k!$ elements, and the entire set of lists has $n!/(n-k)!$ element, then we must have that

$$qk! = n!/(n-k)!\ .$$

Dividing, we solve for q and get an expression for the number of k element subsets of an n element set. In fact, this is how we proved Theorem 1.2.

A principle that helps in learning and understanding mathematics is that if we have a mathematical result that shows a certain symmetry, it often helps our understanding to find a proof that reflects this symmetry. We call this the *Symmetry Principle*.

Principle 1.6 *If a formula has a symmetry (e.g. interchanging two variables doesn't change the result), then a proof that explains this symmetry is likely to give us additional insight into the formula.*

The proof above does not account for the symmetry of the $k!$ term and the $(n-k)!$ term in the expression $\frac{n!}{k!(n-k)!}$. This symmetry arises because choosing a k element subset is equivalent to choosing the $(n-k)$-element subset of elements we don't want. In Exercise 1.4-4, we saw that the binomial coefficient $\binom{n}{k}$ also counts the number of ways to label n objects, say with the labels "in" and "out," so that we have k "ins" and therefore $n-k$ "outs." For each labelling, the k objects that get the label "in" are in our subset. This explains the symmetry in our formula, but it doesn't prove the formula. Here is a new proof that the number of labellings is $n!/k!(n-k)!$ that explains the symmetry.

Suppose we have m ways to assign k blue and $n-k$ red labels to n elements. From each labeling, we can create a number of lists, using the convention of listing the k blue elements first and the remaining $n-k$ red elements last. For example, suppose we are considering the number of ways to label 3 elements blue (and 2 red) from a five element set $\{A, B, C, D, E\}$. Consider the particular labelling in which A, B, and D are labelled blue and C and E are labelled red. Which lists correspond to this labelling? They are

$$\begin{array}{cccccc} ABDCE & ABDEC & ADBCE & ADBEC & BADCE & BADEC \\ BDACE & BDAEC & DABCE & DABEC & DBACE & DBAEC \end{array}$$

that is, all lists in which A, B, and D precede C and E. Since there are 3! ways to arrange A, B, and D, and 2! ways to arrange C and E, by the product principal, there are $3!2! = 12$ lists in which A, B, and D precede C and E. For each of the q ways to construct a labelling, we could find a similar set of 12 lists that are associated with that labelling. Since *every* possible list of 5 elements will appear exactly once via this process, and since there are $5! = 120$ five-element lists overall, we must have by the product principle that

$$q \cdot 12 = 120, \tag{1.14}$$

or that $q = 10$. This agrees with our previous calculations of $\binom{5}{3} = 10$ for the number of ways to label 5 items so that 3 are blue and 2 are red.

Generalizing, we let q be the number of ways to label n objects with k blue labels and $n-k$ red labels. To create the lists associated with a labelling, we list the blue elements first and then the red elements. We can mix the k blue elements among themselves, and we can mix the $n-k$ red elements among themselves, giving us $k!(n-k)!$ lists consisting of first the elements with a blue label followed by the elements with a red label. Since we can choose to label any k elements blue, each of our lists of n distinct elements arises from some labelling in this way. Each such list arises from only one labelling, because two different labellings will have a different first k elements in any list that corresponds to the labelling. Each such list arises only once from a given labelling, because two different lists that correspond to the same labelling differ by a permutation of the first k places or the last $n-k$ places or both. Therefore, by the product principle, $qk!(n-k)!$ is the number of lists we can form with n distinct objects, and this must equal $n!$. This gives us

$$qk!(n-k)! = n!,$$

and division gives us our original formula for q. Recall that our proof of the formula we had in Exercise 1.4-5 did not explain why the product of three factorials appeared in the denominator, it simply proved the formula was correct. With this idea in hand, we could now explain *why* the product in the denominator of the formula in Exercise 1.4-5 for the number of labellings with three labels is what it is, and could generalize this formula to four or more labels.

Equivalence Relations

The process above divided the set of all $n!$ lists of n distinct elements into classes (another word for sets) of lists. In each class, all the lists are mutually equivalent, with respect to labeling with two labels. More precisely, two lists of the n objects are equivalent for defining labellings if we get one from the other by mixing the first k elements among themselves and mixing the last $n-k$ elements among themselves. Relating objects we want to count to sets of lists (so that each object corresponds to an set of equivalent lists) is a technique we can use to solve a wide variety of counting problems. (This is another example of abstraction.)

A relationship that divides a set up into mutually exclusive classes is called an **equivalence relation**.[8] Thus, if

$$S = S_1 \cup S_2 \cup \ldots \cup S_m$$

and $S_i \cap S_j = \emptyset$ for all i and j with $i \neq j$, then the relationship that says any two elements $x \in S$ and $y \in S$ are equivalent if and only if they lie in the same set S_i is an equivalence relation. The sets S_i are called *equivalence classes*, and, as we noted in Section 1.1 the family $S_1, S_2, \ldots, S_m$ is called a **partition** of S. One partition of the set $S = \{a, b, c, d, e, f, g\}$ is $\{a, c\}$, $\{d, g\}$, $\{b, e, f\}$. This partition corresponds to the following (boring) equivalence relation: a and c are equivalent, d and g are equivalent, and b, e, and f are equivalent. A slightly less boring equivalence relation is that two letters are equivalent if typographically, their top and bottom are at the same height. This give the partition $\{a, c, e\}$, $\{b, d\}$, $\{f\}$, $\{g\}$.

Exercise 1.4-1 On the set of integers between 0 and 12 inclusive, define two integers to be related if they have the same remainder on division by 3. Which numbers are related to 0? to 1? to 2? to 3? to 4?. Is this relationship an equivalence relation?

In Exercise 1.4-1, the set of numbers related to 0 is the set $\{0, 3, 6, 9, 12\}$, the set to 1 is $\{1, 4, 7, 10\}$, the set related to 2 is $\{2, 5, 8, 11\}$, the set related to 3 is $\{0, 3, 6, 9, 12\}$, the set related to 4 is $\{1, 4, 7, 10\}$. A little more precisely, a number is related to one of 0, 3, 6, 9, or 12, if and only if it is in the set $\{0, 3, 6, 9, 12\}$, a number is related to 1, 4, 7, or 10 if and only if it is in the set $\{1, 4, 7, 10\}$ and a number is related to 2, 5, 8, or 11 if and only if it is in the set $\{2, 5, 8, 11\}$. Therefore the relationship is an equivalence relation.

The Quotient Principle

In Exercise 1.4-1 the equivalence classes had two different sizes. In the examples of counting labellings and subsets that we have seen so far, all the equivalence classes had the same size. This was very important. The principle we have been using to count subsets and labellings is given in the following theorem. We will call this principle the **Quotient Principle**.

Theorem 1.5 (Quotient Principle) *If an equivalence relation on a p-element set S has q classes each of size r, then $q = p/r$.*

Proof: By the product principle, $p = qr$, and so $q = p/r$. ∎

Another statement of the quotient principle that uses the idea of a partition is

Principle 1.7 (Quotient Principle.) *If we can partition a set of size p into q blocks of size r, then $q = p/r$.*

Returning to our example of 3 blue and 2 red labels, $s = 5! = 120$, $t = 12$ and so by Theorem 1.5,

$$m = \frac{s}{t} = \frac{120}{12} = 10 \ .$$

[8] The usual mathematical approach to equivalence relations, which we shall discuss in the exercises, is different from the one given here. Typically, one sees an equivalence relation defined as a reflexive (everything is related to itself), symmetric (if x is related to y, then y is related to x), and transitive (if x is related to y and y is related to z, then x is related to z) relationship on a set X. Examples of such relationships are equality (on any set), similarity (on a set of triangles), and having the same birthday as (on a set of people). The two approaches are equivalent, and we haven't found a need for the details of the other approach in what we are doing in this course.

Equivalence class counting

We now give several examples of the use of Theorem 1.5.

Exercise 1.4-2 When four people sit down at a round table to play cards, two lists of their four names are equivalent as seating charts if each person has the same person to the right in both lists[9]. (The person to the right of the person in position 4 of the list is the person in position 1). We will use Theorem 1.5 to count the number of possible ways to seat the players. We will take our set S to be the set of all 4-element permutations of the four people, i.e., the set of all lists of the four people.

(a) How many lists are equivalent to a given one?

(b) What are the lists equivalent to ABCD?

(c) Is the relationship of equivalence an equivalence relation?

(d) Use the Quotient Principle to compute the number of equivalence classes, and hence, the number of possible ways to seat the players.

Exercise 1.4-3 We wish to count the number of ways to attach n distinct beads to the corners of a regular n-gon (or string them on a necklace). We say that two lists of the n beads are equivalent if each bead is adjacent to exactly the same beads in both lists. (The first bead in the list is considered to be adjacent to the last.)

- How does this exercise differ from the previous exercise?
- How many lists are in an equivalence class?
- How many equivalence classes are there?

In Exercise 1.4-2, suppose we have named the places at the table north, east, south, and west. Given a list we get an equivalent one in two steps. First we observe that we have four choices of people to sit in the north position. Then there is one person who can sit to this person's right, one who can be next on the right, and one who can be the following on on the right, all determined by the original list. Thus there are exactly four lists equivalent to a given one, including that given one. The lists equivalent to ABCD are ABCD, BCDA, CDAB, and DABC. This shows that two lists are equivalent if and only if we can get one from the other by moving everyone the same number of places to the right around the table (or we can get one from the other moving everyone the same number of places to the left around the table). From this we can see we have an equivalence relation, because each list is in one of these sets of four equivalent lists, and if two lists are equivalent, they are right or left shifts of each other, and we've just observed that all right and left shifts of a given list are in the same class. This means our relationship divides the set of all lists of the four names into equivalence classes each of size four. There are a total of $4! = 24$ lists of four distinct names, and so by Theorem 1.5 we have $4!/4 = 3! = 6$ seating arrangements.

Exercise 1.4-3 is similar in many ways to Exercise 1.4-2, but there is one significant difference. We can visualize the problem as one of dividing lists of n distinct beads up into equivalence classes,

[9]Think of the four places at the table as being called north, east, south, and west, or numbered 1-4. Then we get a list by starting with the person in the north position (position 1), then the person in the east position (position 2) and so on clockwise

but now two lists are equivalent if each bead is adjacent to exactly the same beads in both of them. Suppose we number the vertices of our polygon as 1 through n clockwise. Given a list, we can count the equivalent lists as follows. We have n choices for which bead to put in position 1. Then either of the two beads adjacent to it[10] in the given list can go in position 2. But now, only one bead can go in position 3, because the other bead adjacent to position 2 is already in position 1. We can continue in this way to fill in the rest of the list. For example, with $n = 4$, the lists ABCD, ADCB, BCDA, BADC, CDAB, CBAD, DABC, and DCBA are all equivalent. Notice the first, third , fifth and seventh lists are obtained by shifting the beads around the polygon, as are the second, fourth, sixth and eighth (though in the opposite direction). Also note that the eighth list is the reversal of the first, the third is the reversal of the second, and so on. Rotating a necklace in space corresponds to shifting the letters in the list. Flipping a necklace over in space corresponds to reversing the order of a list. There will always be $2n$ lists we can get by shifting and reversing shifts of a list. The lists equivalent to a given one consist of everything we can get from the given list by rotations and reversals. Thus the relationship of every bead being adjacent to the same beads divides the set of lists of beads into disjoint sets. These sets, which have size $2n$, are the equivalence classes of our equivalence relation. Since there are $n!$ lists, Theorem 1.5 says there are

$$\frac{n!}{2n} = \frac{(n-1)!}{2}$$

bead arrangements.

Multisets

Sometimes when we think about choosing elements from a set, we want to be able to choose an element more than once. For example the set of letters of the word "roof" is $\{f, o, r\}$. However it is often more useful to think of the of the *multiset* of letters, which in this case is $\{\{f, o, o, r\}\}$. We use the double brackets to distinguish a multiset from a set. We can specify a *multiset* chosen from a set S by saying how many times each of its elements occurs. If S is the set of English letters, the "multiplicity" function for roof is given by $m(f) = 1$, $m(o) = 2$, $m(r) = 1$, and $m(\text{letter}) = 0$ for every other letter. In a multiset, order is not important, that is the multiset $\{\{r, o, f, o\}\}$ is equivalent to the multiset $\{\{f, o, o, r\}\}$. We know that this is the case, because they each have the same multiplicity function. We would like to say that the size of $\{\{f, o, o, r\}\}$ is 4, so we define the *size* of a multiset to be the sum of the multiplicities of its elements.

Exercise 1.4-4 Explain how placing k identical books onto the n shelves of a bookcase can be thought of as giving us a k-element multiset of the shelves of the bookcase. Explain how distributing k identical apples to n children can be thought of as giving us a k-element multiset of the children.

In Exercise 1.4-4 we can think of the multiplicity of a bookshelf as the number of books it gets and the multiplicity of a child as the number of apples the child gets. In fact, this idea of distribution of identical objects to distinct recipients gives a great mental model for a multiset chosen from a set S. Namely, to determine a k-element multiset chosen from S form S, we "distribute" k identical objects to the elements of S and the number of objects an element x gets is the multiplicity of x.

[10]Remember, the first and last bead are considered adjacent, so they have two beads adjacent to them.

Notice that it makes no sense to ask for the number of multisets we may choose from a set with n elements, because $\{\{A\}\}$, $\{\{A, A\}\}$, $\{\{A, A, A\}\}$, and so on are infinitely many multisets chosen from the set $\{A\}$. However it does make sense to ask for the number of k-element multisets we can choose from an n-element set. What strategy could we employ to figure out this number? To count k-element subsets, we first counted k-element permutations, and then divided by the number of different permutations of the same set. Here we need an analog of permutations that allows repeats. A natural idea is to consider lists with repeats. After all, one way to describe a multiset is to list it, and there could be many different orders for listing a multiset. However the two element multiset $\{\{A, A\}\}$ can be listed in just one way, while the two element multiset $\{\{A, B\}\}$ can be listed in two ways. When we counted k-element subsets of an n-element set by using the quotient principle, it was essential that each k-element subset corresponded to the same number (namely $k!$) of permutations (lists), because we were using the reasoning behind the quotient principle to do our counting here. So if we hope to use similar reasoning, we can't apply it to lists with repeats because different k-element multisets can correspond to different numbers of lists.

Suppose, however, we could count the number of ways to arrange k distinct books on the n shelves of a bookcase. We can still think of the multiplicity of a shelf as being the number of books on it. However, many different arrangements of distinct books will give us the same multiplicity function. In fact, any way of mixing the books up among themselves that does not change the number of books on each shelf will give us the same multiplicities. But the number of ways to mix the books up among themselves is the number of permutations of the books, namely $k!$. Thus it looks like we have an equivalence relation on the arrangements of distinct books on a bookshelf such that

1. Each equivalence class has $k!$ elements, and
2. There is a bijection between the equivalence classes and k-element multisets of the n shelves.

Thus if we can compute the number of ways to arrange k *distinct* books on the n shelves of a bookcase, we should be able to apply the quotient principle to compute the number of k-element multisets of an n-element set.

The bookcase arrangement problem.

Exercise 1.4-5 We have k books to arrange on the n shelves of a bookcase. The order in which the books appear on a shelf matters, and each shelf can hold all the books. We will assume that as the books are placed on the shelves they are moved as far to the left as they will go so that all that matters is the order in which the books appear and not the actual places where the books sit. When book i is placed on a shelf, it can go between two books already there or to the left or right of all the books on that shelf.

(a) Since the books are distinct, we may think of a first, second, third, etc. book. In how many ways may we place the first book on the shelves?

(b) Once the first book has been placed, in how many ways may the second book be placed?

(c) Once the first two books have been placed, in how many ways may the third book be placed?

(d) Once $i-1$ books have been placed, book i can be placed on any of the shelves to the left of any of the books already there, but there are some additional ways in which it may be placed. In how many ways in total may book i be placed?

(e) In how many ways may k distinct books be place on n shelves in accordance with the constraints above?

Exercise 1.4-6 How many k-element multisets can we choose from an n-element set?

In Exercise 1.4-5 there are n places where the first book can go, namely on the left side of any shelf. Then the next book can go in any of the n places on the far left side of any shelf, or it can go to the right of book one. Thus there are $n+1$ places where book 2 can go. At first, placing book three appears to be more complicated, because we could create two different patterns by placing the first two books. However book 3 could go to the far left of any shelf or to the immediate right of any of the books already there. (Notice that if book 2 and book 1 are on shelf 7 in that order, putting book 3 to the immediate right of book 2 means putting it between book 2 and book 1.) Thus in any case, there are n+2 ways to place book 3. Similarly, once $i-1$ books have been placed, there are $n+i-1$ places where we can place book i. It can go at the far left of any of the n shelves or to the immediate right of any of the $i-1$ books that we have already placed. Thus the number of ways to place k distinct books is

$$n(n+1)(n+2)\cdots(n+k-1)=\prod_{i=1}^{k}(n+i-1)=\prod_{j=0}^{k-1}(n+j)=\frac{(n+k-1)!}{(n-1)!}. \tag{1.15}$$

The specific product that arose in Equation 1.15 is called a *rising factorial power*. It has a notation (also introduced by Don Knuth) analogous to that for the falling factorial notation. Namely, we write

$$n^{\overline{k}}=n(n+1)\cdots(n+k-1)=\prod_{i=1}^{k}(n+i-1).$$

This is the product of k successive numbers beginning with n.

The number of k-element multisets of an n-element set.

We can apply the formula of Exercise 1.4-5 to solve Exercise 1.4-6. We define two bookcase arrangements of k books on n shelves to be equivalent if we get one from the other by permuting the books among themselves. Thus if two arrangements put the same number of books on each shelf they are put into the same class by this relationship. On the other hand, if two arrangements put a different number of books on at least one shelf, they are not equivalent, and therefore they are put into different classes by this relationship. Thus the classes into which this relationship divides the the arrangements are disjoint and partition the set of all arrangements. Each class has $k!$ arrangements in it. The set of all arrangements has $n^{\overline{k}}$ arrangements in it. This leads to the following theorem.

Theorem 1.6 *The number of k-element multisets chosen from an n-element set is*

$$\frac{n^{\overline{k}}}{k!}=\binom{n+k-1}{k}.$$

Proof: The relationship on bookcase arrangements that two arrangements are equivalent if and only if we get one from the other by permuting the books is an equivalence relation. The set of all arrangements has $n^{\overline{k}}$ elements, and the number of elements in an equivalence class is $k!$. By the quotient principle, the number of equivalence classes is $\frac{n^{\overline{k}}}{k!}$. There is a bijection between equivalence classes of bookcase arrangements with k books and multisets with k elements. The second equality follows from the definition of binomial coefficients. ■

The number of k-element multisets chosen from an n-elements is sometimes called the number of *combinations with repetitions* of n elements taken k at a time.

The right-hand side of the formula is a binomial coefficient, so it is natural to ask whether there is a way to interpret choosing a k-element *multi*set from an n-element set as choosing a k-element *sub*set of some different $n + k - 1$-element set. This illustrates an important principle. When we have a quantity that turns our to be equal to a binomial coefficient, it helps our understanding to interpret it as counting the number of ways to choose a subset of an appropriate size from a set of an appropriate size. We explore this idea for multisets in Problem 8 in this section.

Using the quotient principle to explain a quotient

Since the last expression in Equation 1.15 is quotient of two factorials it is natural to ask whether it is counting equivalence classes of an equivalence relation. If so, the set on which the relation is defined has size $(n + k - 1)!$. Thus it might be all lists or permutations of $n + k - 1$ distinct objects. The size of an equivalence class is $(n - 1)!$ and so what makes two lists equivalent might be permuting $n - 1$ of the objects among themselves. Said differently, the quotient principle suggests that we look for an explanation of the formula involving lists of $n + k - 1$ objects, of which $n - 1$ are identical, so that the remaining k elements are distinct. Can we find such an interpretation?

Exercise 1.4-7 In how many ways may we arrange k distinct books and $n - 1$ identical blocks of wood in a straight line?

Exercise 1.4-8 How does Exercise 1.4-7 relate to arranging books on the shelves of a bookcase?

In Exercise 1.4-7, if we tape numbers to the wood so that so that the pieces of wood are distinguishable, there are $(n + k - 1)!$ arrangements of the books and wood. But since the pieces of wood are actually indistinguishable, $(n - 1)!$ of these arrangements are equivalent. Thus by the quotient principle there are $(n + k - 1)!/(n - 1)!$ arrangements. Such an arrangement allows us to put the books on the shelves as follows: put all the books before the first piece of wood on shelf 1, all the books between the first and second on shelf 2, and so on until you put all the books after the last piece of wood on shelf n.

Important Concepts, Formulas, and Theorems

1. *Symmetry Principle.* If we have a mathematical result that shows a certain symmetry, it often helps our understanding to find a proof that reflects this symmetry.

2. *Partition.* Given a set S of items, a *partition* of S consists of m sets $S_1, S_2, \ldots, S_m$, sometimes called *blocks* so that $S_1 \cup S_2 \cup \cdots \cup S_m = S$ and for each i and j with $i \neq j$, $S_i \cap S_j = \emptyset$.

3. *Equivalence relation. Equivalence class.* A relationship that partitions a set up into mutually exclusive classes is called an **equivalence relation**. Thus if $S = S_1 \cup S_2 \cup \ldots \cup S_m$ is a partition of S, the relationship that says any two elements $x \in S$ and $y \in S$ are equivalent if and only if they lie in the same set S_i is an equivalence relation. The sets S_i are called *equivalence classes*

4. *Quotient principle.* The **quotient principle** says that if we can partition a set of p objects up into q classes of size r, then $q = p/r$. Equivalently, if an equivalence relation on a set of size p has q equivalence classes of size r, then $q = p/r$. The quotient principle is frequently used for counting the number of equivalence classes of an equivalence relation. When we have a quantity that is a quotient of two others, it is often helpful to our understanding to find a way to use the quotient principle to explain why we have this quotient.

5. *Multiset.* A multiset is similar to a set except that each item can appear multiple times. We can specify a *multiset* chosen from a set S by saying how many times each of its elements occurs.

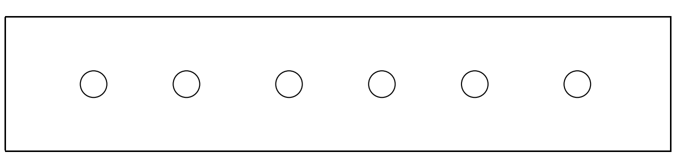
6. *Choosing k-element multisets.* The number of k-element multisets that can be chosen from an n-element set is
$$\frac{(n+k-1)!}{k!(n-1)!} = \binom{n+k-1}{k}.$$
This is sometimes called the formula for "combinations with repetitions."

7. *Interpreting binomial coefficients.* When we have a quantity that turns out to be a binomial coefficient (or some other formula we recognize) it is often helpful to our understanding to try to interpret the quantity as the result of choosing a subset of a set (or doing whatever the formula that we recognize counts.)

Problems

1. In how many ways may n people be seated around a round table? (Remember, two seating arrangements around a round table are equivalent if everyone is in the same position relative to everyone else in both arrangements.)

2. In how many ways may we embroider n circles of different colors in a row (lengthwise, equally spaced, and centered halfway between the top and bottom edges) on a scarf (as follows)?



3. Use binomial coefficients to determine in how many ways three identical red apples and two identical golden apples may be lined up in a line. Use equivalence class counting (in particular, the quotient principle) to determine the same number.

4. Use multisets to determine the number of ways to pass out k identical apples to n children.

5. In how many ways may n men and n women be seated around a table alternating gender? (Use equivalence class counting!!)

6. In how many ways may we pass out k identical apples to n children if each child must get at least one apple?

7. In how many ways may we place k distinct books on n shelves of a bookcase (all books pushed to the left as far as possible) if there must be at least one book on each shelf?

8. The formula for the number of multisets is $(n+k-1)!$ divided by a product of two other factorials. We seek an explanation using the quotient principle of why this counts multisets. The formula for the number of multisets is also a binomial coefficient, so it should have an interpretation involving choosing k items from $n+k-1$ items. The parts of the problem that follow lead us to these explanations.

   (a) In how many ways may we place k red checkers and $n-1$ black checkers in a row?

   (b) How can we relate the number of ways of placing k red checkers and $n-1$ black checkers in a row to the number of k-element multisets of an n-element set, say the set $\{1, 2, \ldots, n\}$ to be specific?

   (c) How can we relate the choice of k items out of $n+k-1$ items to the placement of red and black checkers as in the previous parts of this problem?

9. How many solutions to the equation $x_1 + x_2 + \cdots x_n = k$ are there with each $x_i \geq 0$?

10. How many solutions to the equation $x_1 + x_2 + \cdots x_n = k$ are there with each $x_i > 0$?

11. In how many ways may n red checkers and $n+1$ black checkers be arranged in a circle? (This number is a famous number called a *Catalan number*.)

12. A standard notation for the number of partitions of an n element set into k classes is $S(n,k)$. $S(0,0)$ is 1, because technically the empty family of subsets of the empty set is a partition of the empty set, and $S(n,0)$ is 0 for $n > 0$, because there are no partitions of a nonempty set into no parts. $S(1,1)$ is 1.

    (a) Explain why $S(n,n)$ is 1 for all $n > 0$. Explain why $S(n,1)$ is 1 for all $n > 0$.

    (b) Explain why, for $1 < k < n$, $S(n,k) = S(n-1,k-1) + kS(n-1,k)$.

    (c) Make a table like our first table of binomial coefficients that shows the values of $S(n,k)$ for values of n and k ranging from 1 to 6.

13. You are given a square, which can be rotated 90 degrees at a time (i.e. the square has four orientations). You are also given two red checkers and two black checkers, and you will place each checker on one corner of the square. How many lists of four letters, two of which are R and two of which are B, are there? Once you choose a starting place on the square, each list represents placing checkers on the square in clockwise order. Consider two lists to be equivalent if they represent the same arrangement of checkers at the corners of the square, that is, if one arrangement can be rotated to create the other one. Write down the equivalence classes of this equivalence relation. Why can't we apply Theorem 1.5 to compute the number of equivalence classes?

14. The terms “reflexive”, “symmetric” and “transitive” were defined in Footnote 2. Which of these properties is satisfied by the relationship of “greater than?” Which of these properties is satisfied by the relationship of “is a brother of?” Which of these properties is satisfied by “is a sibling of?” (You are not considered to be your own brother or your own sibling). How about the relationship “is either a sibling of or is?”

    a Explain why an equivalence relation (as we have defined it) is a reflexive, symmetric, and transitive relationship.

    b Suppose we have a reflexive, symmetric, and transitive relationship defined on a set S. For each x is S, let $S_x = \{y|y \text{ is related to } x\}$. Show that two such sets S_x and S_y are either disjoint or identical. Explain why this means that our relationship is an equivalence relation (as defined in this section of the notes, not as defined in the footnote).

    c Parts b and c of this problem prove that a relationship is an equivalence relation if and only if it is symmetric, reflexive, and transitive. Explain why. (A short answer is most appropriate here.)

15. Consider the following C++ function to compute $\binom{n}{k}$.

```
int pascal(int n, int k)
{
  if (n < k)
    {

      cout << "error: n<k" << endl;
      exit(1);
    }

  if ( (k==0) || (n==k))
    return 1;


  return  pascal(n-1,k-1) + pascal(n-1,k);
}
```

    Enter this code and compile and run it (you will need to create a simple main program that calls it). Run it on larger and larger values of n and k, and observe the running time of the program. It should be surprisingly slow. (Try computing, for example, $\binom{30}{15}$.) Why is it so slow? Can you write a different function to compute $\binom{n}{k}$ that is *significantly faster*? Why is your new version faster? (Note: an exact analysis of this might be difficult at this point in the course; it will be easier later. However, you should be able to figure out roughly why this version is so much slower.)

16. Answer each of the following questions with either n^k, $n^{\underline{k}}$, $\binom{n}{k}$, or $\binom{n+k-1}{k}$.

    (a) In how many ways can k different candy bars be distributed to n people (with any person allowed to receive more than one bar)?

    (b) In how many ways can k different candy bars be distributed to n people (with nobody receiving more than one bar)?

(c) In how many ways can k identical candy bars distributed to n people (with any person allowed to receive more than one bar)?

(d) In how many ways can k identical candy bars distributed to n people (with nobody receiving more than one bar)?

(e) How many one-to-one functions f are there from $\{1, 2, \ldots, k\}$ to $\{1, 2, \ldots, n\}$?

(f) How many functions f are there from $\{1, 2, \ldots, k\}$ to $\{1, 2, \ldots, n\}$?

(g) In how many ways can one choose a k-element subset from an n-element set?

(h) How many k-element multisets can be formed from an n-element set?

(i) In how many ways can the top k ranking officials in the US government be chosen from a group of n people?

(j) In how many ways can k pieces of candy (not necessarily of different types) be chosen from among n different types?

(k) In how many ways can k children each choose one piece of candy (all of different types) from among n different types of candy?

Chapter 2

Cryptography and Number Theory

2.1 Cryptography and Modular Arithmetic

Introduction to Cryptography

For thousands of years people have searched for ways to send messages secretly. There is a story that, in ancient times, a king needed to send a secret message to his general in battle. The king took a servant, shaved his head, and wrote the message on his head. He waited for the servant's hair to grow back and then sent the servant to the general. The general then shaved the servant's head and read the message. If the enemy had captured the servant, they presumably would not have known to shave his head, and the message would have been safe.

Cryptography is the study of methods to send and receive secret messages. In general, we have a *sender* who is trying to send a message to a *receiver*. There is also an *adversary*, who wants to steal the message. We are successful if the sender is able to communicate a message to the receiver without the adversary learning what that message was.

Cryptography has remained important over the centuries, used mainly for military and diplomatic communications. Recently, with the advent of the internet and electronic commerce, cryptography has become vital for the functioning of the global economy, and is something that is used by millions of people on a daily basis. Sensitive information such as bank records, credit card reports, passwords, or private communication, is (and should be) *encrypted*—modified in such a way that, hopefully, it is only understandable to people who should be allowed to have access to it, and *undecipherable* to others.

Undecipherability by an adversary is, of course, a difficult goal. No code is completely undecipherable. If there is a printed "codebook," then the adversary can always steal the codebook, and no amount of mathematical sophistication can prevent this possibility. More likely, an adversary may have extremely large amounts of computing power and human resources to devote to trying to crack a code. Thus our notion of security is tied to computing power—a code is only as safe as the amount of computing power needed to break it. If we design codes that seem to need exceptionally large amounts of computing power to break, then we can be relatively confident in their security.

Private Key Cryptography

Traditional cryptography is known as *private key cryptography.* The sender and receiver agree in advance on a *secret code*, and then send messages using that code. For example, one of the oldest codes is known as a *Caesar cipher*. In this code, the letters of the alphabet are shifted by some fixed amount. Typically, we call the original message the *plaintext* and the encoded text the *ciphertext.* An example of a Caesar cipher would be the following code:

```
plaintext  A B C D E F G H I J K L M N O P Q R S T U V W X Y Z
ciphertext E F G H I J K L M N O P Q R S T U V W X Y Z A B C D .
```

Thus if we wanted to send the plaintext message

ONE IF BY LAND AND TWO IF BY SEA ,

we would send the ciphertext

SRI MJ FC PERH ERH XAS MJ FC WIE .

A Caeser cipher is especially easy to implement on a computer using a scheme known as arithmetic mod 26. The symbolism

$$m \bmod n$$

means the remainder we get when we divide m by n. A bit more precisely we can give the following definition.

Definition 2.1 *For integers m and n, $m \bmod n$ is the smallest nonnegative integer r such that*

$$m = nq + r \tag{2.1}$$

for some integer q.

We will refer to the fact that $m \bmod n$ is always well defined as Euclid's division theorem. The proof appears in the next section.[1]

Theorem 2.1 (Euclid's division theorem) *For every integer m and positive integer n, there exist unique integers q and r such that $m = nq + r$ and $0 \le r < n$.*

Exercise 2.1-1 Use The definition of $m \bmod n$ to compute $10 \bmod 7$ and $-10 \bmod 7$. What are q and r in each case? Does $(-m) \bmod n = -(m \bmod n)$?

[1] In an unfortunate historical evolution of terminology, the fact that for every nonnegative integer m and positive integer n, there exist unique nonnegative integers q and r such that $m = nq + r$ and $r < n$ is called "Euclid's algorithm." In modern language we would call this "Euclid's Theorem" instead. While it seems obvious that there is such a smallest nonnegative integer r and that there is exactly one such pair q, r with $r < n$, a technically complete study would derive these facts from the basic axioms of number theory, just as "obvious" facts of geometry are derived from the basic axioms of geometry. The reasons why mathematicians take the time to derive such obvious facts from basic axioms is so that everyone can understand exactly what we are assuming as the foundations of our subject; as the "rules of the game" in effect.

Exercise 2.1-2 Using 0 for A, 1 for B, and so on, let the numbers from 0 to 25 stand for the letters of the alphabet. In this way, convert a message to a sequence of strings of numbers. For example SEA becomes 18 4 0. What does (the numerical representation of) this word become if we shift every letter two places to the right? What if we shift every letter 13 places to the right? How can you use the idea of $m \bmod n$ to implement a Caeser cipher?

Exercise 2.1-3 Have someone use a Caeser cipher to encode a message of a few words in your favorite natural language, without telling you how far they are shifting the letters of the alphabet. How can you figure out what the message is? Is this something a computer could do quickly?

In Exercise 2.1-1, $10 = 7(1)+3$ and so $10 \bmod 7$ is 3, while $-10 = 7(-2)+4$ and so $-10 \bmod 7$ is 4. These two calculations show that $(-m) \bmod n = -(m \bmod n)$ is not necessarily true. Note that $-3 \bmod 7$ is 4 also. Furthermore, $-10 + 3 \bmod 7 = 0$, suggesting that -10 is essentially the same as -3 when we are considering integers mod 7.

In Exercise 2.1-2, to shift each letter two places to the right, we replace each number n in our message by $(n+2) \bmod 26$, so that SEA becomes 20 8 2. To shift 13 places to the right, we replace each number n in our message with $(n + 13) \bmod 26$ so that SEA becomes 5 17 13. Similarly to implement a shift of s places, we replace each number n in our message by $(n + s) \bmod 26$. Since most computer languages give us simple ways to keep track of strings of numbers and a "mod function," it is easy to implement a Caeser cipher on a computer.

Exercise 2.1-3 considers the complexity of encoding, decoding and cracking a Ceasar cipher. Even by hand, it is easy for the sender to encode the message, and for the receiver to decode the message. The disadvantage of this scheme is that it is also easy for the adversary to just try the 26 different possible Caesar ciphers and decode the message. (It is very likely that only one will decode into plain English.) Of course, there is no reason to use such a simple code; we can use any arbitrary permutation of the alphabet as the ciphertext, e.g.

```
plaintext  A B C D E F G H I J K L M N O P Q R S T U V W X Y Z
ciphertext H D I E T J K L M X N Y O P F Q R U V W G Z A S B C
```

If we encode a short message with a code like this, it would be hard for the adversary to decode it. However, with a message of any reasonable length (greater than about 50 letters), an adversary with a knowledge of the statistics of the English language can easily crack the code. (These codes appear in many newspapers and puzzle books under the name cryptograms. Many people are able to solve these puzzles, which is compelling evidence of the lack of security in such a code.)

We do not have to use simple mappings of letters to letters. For example, our coding algorithm can be to

- take three consecutive letters,
- reverse their order,
- interpret each as a base 26 integer (with A=0; B=1, etc.),
- multiply that number by 37,

- add 95 and then
- convert that number to base 8.

We continue this processing with each block of three consecutive letters. We append the blocks, using either an 8 or a 9 to separate the blocks. When we are done, we reverse the number, and replace each digit 5 by two 5's. Here is an example of this method:

```
plaintext: ONEIFBYLANDTWOIFBYSEA

block and reverse: ENO  BFI   ALY     TDN   IOW     YBF    AES
base 26 integer:  3056  814   310    12935  5794   16255   122
*37 +95 base 8: 335017 73005 26455 1646742 642711 2226672 11001
appended      : 335017873005926455916467429642711822266728110001
reverse, 5rep : 10011827662228117246924764619555546295500378710533
```

As Problem 20 shows, a receiver who knows the code can decode this message. Furthermore, a casual reader of the message, without knowledge of the encryption algorithm, would have no hope of decoding the message. So it seems that with a complicated enough code, we can have secure cryptography. Unfortunately, there are at least two flaws with this method. The first is that if the adversary learns, somehow, what the code is, then she can easily decode it. Second, if this coding scheme is repeated often enough, and if the adversary has enough time, money and computing power, this code could be broken. In the field of cryptography, some entities have all these resources (such as a government, or a large corporation). The infamous German Enigma code is an example of a much more complicated coding scheme, yet it was broken and this helped the Allies win World War II. (The reader might be interested in looking up more details on this; it helped a lot in breaking the code to have a stolen Enigma machine, though even with the stolen machine, it was not easy to break the code.) In general, any scheme that uses a *codebook*, a secretly agreed upon (possibly complicated) code, suffers from these drawbacks.

Public-key Cryptosystems

A *public-key* cryptosystem overcomes the problems associated with using a codebook. In a public-key cryptosystem, the sender and receiver (often called *Alice* and *Bob* respectively) don't have to agree in advance on a secret code. In fact, they each publish part of their code in a public directory. Further, an adversary with access to the encoded message and the public directory still cannot decode the message.

More precisely, Alice and Bob will each have two keys, a *public key* and a *secret key*. We will denote Alice's public and secret keys as KP_A and KS_A and Bob's as KP_B and KS_B. They each keep their secret keys to themselves, but can publish their public keys and make them available to anyone, including the adversary. While the key published is likely to be a symbol string of some sort, the key is used in some standardized way (we shall see examples soon) to create a function from the set $\mathcal{D}$ of possible messages onto itself. (In complicated cases, the key might be the actual function). We denote the functions associated with KS_A, KP_A, KS_B and KP_B by

S_A, P_A, S_B, and P_B, respectively. We require that the public and secret keys are chosen so that the corresponding functions are inverses of each other, i.e for any message $M \in \mathcal{D}$ we have that

$$M = S_A(P_A(M)) \quad = \quad P_A(S_A(M)), \text{ and} \tag{2.2}$$
$$M = S_B(P_B(M)) \quad = \quad P_B(S_B(M)). \tag{2.3}$$

We also assume that, for Alice, S_A and P_A are easily computable. However, it is essential that *for everyone except Alice, S_A is hard to compute, even if you know P_A*. At first glance, this may seem to be an impossible task, Alice creates a function P_A, that is public and easy to compute for everyone, yet this function has an inverse, S_A, that is hard to compute for everyone except Alice. It is not at all clear how to design such a function. In fact, when the idea for public key cryptography was proposed (by Diffie and Hellman[2]), no one knew of any such functions. The first complete public-key cryptosystem is the now-famous RSA cryptosystem, widely used in many contexts. To understand how such a cryptosystem is possible requires some knowledge of number theory and computational complexity. We will develop the necessary number theory in the next few sections.

Before doing so, let us just assume that we have such a function and see how we can make use of it. If Alice wants to send Bob a message M, she takes the following two steps:

1. Alice obtains Bob's public key P_B.

2. Alice applies Bob's public key to M to create ciphertext $C = P_B(M)$.

Alice then sends C to Bob. Bob can decode the message by using his secret key to compute $S_B(C)$ which is identical to $S_B(P_B(M))$, which by (2.3) is identical to M, the original message. The beauty of the scheme is that even if the adversary has C and knows P_B, she cannot decode the message without S_B, since S_B is a secret that only Bob has. Even though the adversary knows that S_B is the inverse of P_B, the adversary cannot easily compute this inverse.

Since it is difficult, at this point, to describe an example of a public key cryptosystem that is hard to decode, we will give an example of one that is easy to decode. Imagine that our messages are numbers in the range 1 to 999. Then we can imagine that Bob's public key yields the function P_B given by $P_B(M) = rev(1000 - M)$, where $rev()$ is a function that reverses the digits of a number. So to encrypt the message 167, Alice would compute $1000 - 167 = 833$ and then reverse the digits and send Bob $C = 338$. In this case $S_B(C) = 1000 - rev(C)$, and Bob can easily decode. This code is not secure, since if you know P_B, you can figure out S_B. The challenge is to design a function P_B so that even if you know P_B and $C = P_B(M)$, it is exceptionally difficult to figure out what M is.

Arithmetic modulo n

The RSA encryption scheme is built upon the idea of arithmetic mod n, so we introduce this arithmetic now. Our goal is to understand how the basic arithmetic operations, addition, subtraction, multiplication, division, and exponentiation behave when all arithmetic is done mod n. As we shall see, some of the operations, such as addition, subtraction and multiplication, are straightforward to understand. Others, such as division and exponentiation, behave very differently than they do for normal arithmetic.

[2]Whitfield Diffie and Martin Hellman. "New directions in cryptography" *IEEE Transactions on Information Theory*, **IT-22**(6) pp 644-654, 1976.

Exercise 2.1-4 Compute $21 \bmod 9$, $38 \bmod 9$, $(21 \cdot 38) \bmod 9$, $(21 \bmod 9) \cdot (38 \bmod 9)$, $(21 + 38) \bmod 9$, $(21 \bmod 9) + (38 \bmod 9)$.

Exercise 2.1-5 True or false: $i \bmod n = (i + 2n) \bmod n$; $i \bmod n = (i - 3n) \bmod n$

In Exercise 2.1-4, the point to notice is that

$$(21 \cdot 38) \bmod 9 = (21 \bmod 9)(38 \bmod 9)$$

and

$$(21 + 38) \bmod 9 = (21 \bmod 9) + (38 \bmod 9).$$

These equations are very suggestive, though the general equations that they first suggest aren't true! As we shall soon see, some closely related equations are true.

Exercise 2.1-5 is true in both cases, as adding multiples of n to i does not change the value of $i \bmod n$. In general, we have

Lemma 2.2 $i \bmod n = (i + kn) \bmod n$ *for any integer* k.

Proof: By Theorem 2.1, for unique integers q and r, with $0 \le r < n$, we have

$$i = nq + r. \tag{2.4}$$

Adding kn to both sides of Equation 2.4, we obtain

$$i + kn = n(q + k) + r. \tag{2.5}$$

Applying the definition of $i \bmod n$ to Equation 2.4, we have that $r = i \bmod n$ and applying the same definition to Equation 2.5 we have that $r = (i + kn) \bmod n$. The lemma follows. ■

Now we can go back to the equations of Exercise 2.1-4; the correct versions are stated below. Informally, we are showing if we have a computation involving addition and multiplication, and we plan to take the end result mod n, then we are free to take any of the intermediate results mod n also.

Lemma 2.3

$$\begin{aligned}(i + j) \bmod n &= [i + (j \bmod n)] \bmod n \\ &= [(i \bmod n) + j] \bmod n \\ &= [(i \bmod n) + (j \bmod n)] \bmod n\end{aligned}$$

$$\begin{aligned}(i \cdot j) \bmod n &= [i \cdot (j \bmod n)] \bmod n \\ &= [(i \bmod n) \cdot j] \bmod n \\ &= [(i \bmod n) \cdot (j \bmod n)] \bmod n\end{aligned}$$

Proof: We prove the first and last terms in the sequence of equations for plus are equal; the other equalities for plus follow by similar computations. The proofs of the equalities for products are similar.

By Theorem 2.1, we have that for unique integers q_1 and q_2,

$$i = (i \bmod n) + q_1 n \text{ and } j = (j \bmod n) + q_2 n.$$

Then adding these two equations together mod n, and using Lemma 2.2, we obtain

$$\begin{aligned}
(i+j) \bmod n &= [(i \bmod n) + q_1 n + (j \bmod n) + q_2 n)] \bmod n \\
&= [(i \bmod n) + (j \bmod n) + n(q_1 + q_2)] \bmod n \\
&= [(i \bmod n) + (j \bmod n)] \bmod n.
\end{aligned}$$

■

We now introduce a convenient notation for performing modular arithmetic. We will use the notation Z_n to represent the integers $0, 1, \ldots, n-1$ together with a redefinition of addition, which we denote by $+_n$, and a redefinition of multiplication, which we denote $\cdot_n$. The redefinitions are:

$$i +_n j = (i + j) \bmod n \tag{2.6}$$

$$i \cdot_n j = (i \cdot j) \bmod n \tag{2.7}$$

We will use the expression "$x \in Z_n$" to mean that x is a variable that can take on any of the integral values between 0 and $n-1$. In addition, $x \in Z_n$ is a signal that if we do algebraic operations with x, we are will use $+_n$ and $\cdot_n$ rather than the usual addition and multiplication. In ordinary algebra it is traditional to use letters near the beginning of the alphabet to stand for constants; that is, numbers that are fixed throughout our problem and would be known in advance in any one instance of that problem. This allows us to describe the solution to many different variations of a problem all at once. Thus we might say "For all integers a and b, there is one and only one integer x that is a solution to the equation $a + x = b$, namely $x = b - a$." We adopt the same system for Z_n. When we say "Let a be a member of Z_n," we mean the same thing as "Let a be an integer between 0 and $n-1$," but we are also signaling that in equations involving a, we will use $+_n$ and $\cdot_n$.

We call these new operations addition mod n and multiplication mod n. We must now verify that all the "usual" rules of arithmetic that normally apply to addition and multiplication still apply with $+_n$ and $\cdot_n$. In particular, we wish to verify the commutative, associative and distributive laws.

Theorem 2.4 *Addition and multiplication mod n satisfy the commutative and associative laws, and multiplication distributes over addition.*

Proof: Commutativity follows immediately from the definition and the commutativity of ordinary addition and multiplication. We prove the associative law for addition in the following equations; the other laws follow similarly.

$$\begin{aligned}
a +_n (b +_n c) &= (a + (b +_n c)) \bmod n && \text{(Equation 2.6)} \\
&= (a + ((b + c) \bmod n)) \bmod n && \text{(Equation 2.6)}
\end{aligned}$$

$$
\begin{aligned}
&= (a + (b + c)) \bmod n && \text{(Lemma 2.3)} \\
&= ((a + b) + c) \bmod n && \text{(Associative law for ordinary sums)} \\
&= ((a + b) \bmod n + c) \bmod n && \text{(Lemma 2.3)} \\
&= ((a +_n b) + c) \bmod n && \text{(Equation 2.6)} \\
&= (a +_n b) +_n c && \text{(Equation 2.6).}
\end{aligned}
$$

■

Notice that $0 +_n i = i$, $1 \cdot_n i = i$, (these equations are called the *additive identity properties* and the *multiplicative identity* properties) and $0 \cdot_n i = 0$, so we can use 0 and 1 in algebraic expressions in Z_n (which we may also refer to as agebraic expressions mod n) as we use them in ordinary algebraic expressions. We use $a -_n b$ to stand for $a +_n (-b)$.

We conclude this section by observing that repeated applications of Lemma 2.3 and Theorem 2.4 are useful when computing sums or products mod n in which the numbers are large. For example, suppose you had m integers $x_1, \ldots, x_m$ and you wanted to compute $(\sum_{j=1}^{m} x_i) \bmod n$. One natural way to do so would be to compute the sum, and take the result modulo n. However, it is possible that, on the computer that you are using, even though $(\sum_{j=1}^{m} x_i) \bmod n$ is a number that can be stored in an integer, and each x_i can be stored in an integer, $\sum_{j=1}^{m} x_i$ might be too large to be stored in an integer. (Recall that integers are typically stored as 4 or 8 bytes, and thus have a maximum value of roughly 2×10^9 or 9×10^{18}.) Lemma 2.3 tells us that if we are computing a result mod n, we may do all our calculations in Z_n using $+_n$ and $\cdot_n$, and thus never computing an integer that has significantly more digits than any of the numbers we are working with.

Cryptography using addition mod n

One natural way to use addition of a number a mod n in encryption is first to convert the message to a sequence of digits—say concatenating all the ASCII codes for all the symbols in the message—and then simply add a to the message mod n. Thus $P(M) = M +_n a$ and $S(C) = C +_n (-a) = C -_n a$. If n happens to be larger than the message in numerical value, then it is simple for someone who knows a to decode the encrypted message. However an adversary who sees the encrypted message has no special knowledge and so unless a was ill chosen (for example having all or most of the digits be zero would be a silly choice) the adversary who knows what system you are using, even including the value of n, but does not know a, is essentially reduced to trying all possible a values. (In effect adding a appears to the adversary much like changing digits at random.) Because you use a only once, there is virtually no way for the adversary to collect any data that will aid in guessing a. Thus, if only you and your intended recipient know a, this kind of encryption is quite secure: guessing a is just as hard as guessing the message.

It is possible that once n has been chosen, you will find you have a message which translates to a larger number than n. Normally you would then break the message into segments, each with no more digits than n, and send the segments individually. It might seem that as long as you were not sending a large number of segments, it would still be quite difficult for your adversary to guess a by observing the encrypted information. However if your adversary knew n but not a and knew you were adding a mod n, he or she could take two messages and subtract them in Z_n, thus getting the difference of two unencrypted messages. (In Problem 13 we ask you to explain why, even if your adversary didn't know n, but just believed you were adding some secret number a mod some other secret number n, she or he could use three encoded messages to find three differences in the integers, instead of Z_n, one of which was the difference of two messages.) This difference could contain valuable information for your adversary.[3] And if your adversary could trick you into sending just one message z that he or she knows, intercepting the message and subtracting z would give your adversary a. Thus adding a mod n is not an encoding method you would want to use more than once.

Cryptography using multiplication mod n

We will now explore whether multiplication is a good method for encryption. In particular, we could encrypt by multiplying a message (mod n) by a prechosen value a. We would then expect to decrypt by "dividing" by a. What exactly does division mod a mean? Informally, we think of division as the "inverse" of multiplication, that is, if we take a number x, multiply by a and then divide by a, we should get back x. Clearly, with normal arithmetic, this is the case. However, with modular arithmetic, division is trickier.

Exercise 2.1-6 One possibility for encryption is to take a message x and compute $a \cdot_n x$, for some value a, that the sender and receiver both know. You could then decrypt by doing division by a in Z_n if you knew how to divide in Z_n. How well does this work? In particular, consider the following three cases. First, consider $n = 12$ and $a = 4$ and $x = 3$. Second, consider $n = 12$ and $a = 3$ and $x = 6$. Third, consider $n = 12$ and $a = 5$ and $x = 7$. In each case, ask if your recipient, knowing a, could figure out what the message x is.

When we encoded a message by adding a in Z_n, we could decode the message simply by subtracting a in Z_n. However, this method had significant disadvantages, even if our adversary did not know n. Suppose that instead of encoding by adding a mod n, we encoded by multiplying by a mod n. (This doesn't give us a great secret key cryptosystem, but it illustrates some key points.) By analogy, if we encode by multiplying by a in Z_n, we would expect to decode by dividing by a in Z_n. However, Exercise 2.1-6 shows that division in Z_n doesn't always make very much sense. Suppose your value of n was 12 and the value of a was 4. You send the message 3 as $4 \cdot_{12} 3 = 0$. Thus you send the encoded message 0. Now your recipient sees 0, and says the message might have been 0; after all, $4 \cdot_{12} 0 = 0$. On the other hand, $4 \cdot_{12} 3 = 0$, $4 \cdot_{12} 6 = 0$, and $4 \cdot_{12} 9 = 0$ as well. Thus your recipient has four different choices for the original message, which is almost as bad as having to guess the original message itself!

It might appear that special problems arose because the encoded message was 0, so the next question in Exercise 2.1-6 gives us an encoded message that is not 0. Suppose that $a = 3$ and $n = 12$. Now we encode the message 6 by computing $3 \cdot_{12} 6 = 6$. Straightforward calculation shows that $3 \cdot_{12} 2 = 6$, $3 \cdot_{12} 6 = 6$, and $3 \cdot_{12} 10 = 6$. Thus, the message 6 can be decoded in three possible ways, as 2, 6, or 10.

The final question in Exercise 2.1-6 provides some hope. Let $a = 5$ and $n = 12$. The message is 7 is encoded as $5 \cdot_{12} 7 = 11$. Simple checking of $5 \cdot_{12} 1$, $5 \cdot_{12} 2$, $5 \cdot_{12} 3$, and so on shows that 7 is

[3] If each segement of a message were equally likely to be any number between 0 and n, and if any second (or third, etc.) segment were equally likely to follow any first segement, then knowing the difference between two segments would yield no information about the two segments. However, because language is structured and most information is structured, these two conditions are highly unlikely to hold, in which case your adversary could apply structural knowledge to deduce information about your two messages from their difference.

the unique solution in Z_{12} to the equation $5 \cdot_{12} x = 11$. Thus in this case we can correctly decode the message.

One key point that this example shows is that our system of encrypting messages must be one-to-one. That is, each unencrypted message must correspond to a different encrypted message.

As we shall see in the next section, the kinds of problems we had in Exercise 2.1-6 happen only when a and n have a common divisor that is greater than 1. Thus, when a and n have no common factors greater than one, all our receiver needs to know is how to divide by a in Z_n, and she can decrypt our message. If you don't now know how to divide by a in Z_n, then you can begin to understand the idea of public key cryptography. The message is there for anyone who knows how to divide by a to find, but if nobody but our receiver can divide by a, we can tell everyone what a and n are and our messages will still be secret. That is the second point our system illustrates. If we have some knowledge that nobody else has, such as how to divide by a mod n, then we have a possible public key cryptosystem. As we shall soon see, dividing by a is not particularly difficult, so a better trick is needed for public key cryptography to work.

Important Concepts, Formulas, and Theorems

1. *Cryptography* is the study of methods to send and receive secret messages.
   (a) The *sender* wants to send a message to a *receiver*.
   (b) The *adversary* wants to steal the message.
   (c) In *private key cryptography*, the sender and receiver agree in advance on a *secret code*, and then send messages using that code.
   (d) In *public key cryptography*, the encoding method can be published. Each person has a *public key* used to encrypt messages and a *secret key* used to encrypt an encrypted message.
   (e) The original message is called the *plaintext*.
   (f) The encoded text is called the *ciphertext*.
   (g) A *Caesar cipher* is one in which each letter of the alphabet is shifted by a fixed amount.
2. *Euclid's Division Theorem*. For every integer m and positive integer n, there exist unique integers q and r such that $m = nq + r$ and $0 \le r < n$. By definition, r is equal to $m \bmod n$.
3. *Adding multiples of n does not change values mod n*. That is, $i \bmod n = (i + kn) \bmod n$ for any integer k.
4. *Mods (by n) can be taken anywhere in calculation, so long as we take the final result mod n*.

$$\begin{aligned}(i+j) \bmod n &= [i + (j \bmod n)] \bmod n \\ &= [(i \bmod n) + j] \bmod n \\ &= [(i \bmod n) + (j \bmod n)] \bmod n\end{aligned}$$

$$\begin{aligned}(i \cdot j) \bmod n &= [i \cdot (j \bmod n)] \bmod n \\ &= [(i \bmod n) \cdot j] \bmod n \\ &= [(i \bmod n) \cdot (j \bmod n)] \bmod n\end{aligned}$$

5. *Commutative, associative and distributive laws.* Addition and multiplication mod n satisfy the commutative and associative laws, and multiplication distributes over addition.

6. Z_n. We use the notation Z_n to represent the integers $0, 1, \ldots, n-1$ together with a redefinition of addition, which we denote by $+_n$, and a redefinition of multiplication, which we denote $\cdot_n$. The redefinitions are:

$$\begin{aligned} i +_n j &= (i + j) \bmod n \\ i \cdot_n j &= (i \cdot j) \bmod n \end{aligned}$$

We use the expression "$x \in Z_n$" to mean that x is a variable that can take on any of the integral values between 0 and $n-1$, and that in algebraic expressions involving x we will use $+_n$ and $\cdot_n$. We use the expression $a \in Z_n$ to mean that a is a constant between 0 and $n-1$, and in algebraic expressions involving a we will use $+_n$ and $\cdot_n$.

Problems

1. What is 14 mod 9? What is -1 mod 9? What is -11 mod 9?

2. Encrypt the message HERE IS A MESSAGE using a Caeser cipher in which each letter is shifted three places to the right.

3. Encrypt the message HERE IS A MESSAGE using a Caeser cipher in which each letter is shifted three places to the left.

4. How many places has each letter been shifted in the Caesar cipher used to encode the message XNQQD RJXXFLJ?

5. What is $16 +_{23} 18$? What is $16 \cdot_{23} 18$?

6. A short message has been encoded by converting it to an integer by replacing each "a" by 1, each "b" by 2, and so on, and concatenating the integers. The result had six or fewer digits. An unknown number a was added to the message mod 913,647, giving 618,232. Without the knowledge of a, what can you say about the message? With the knowledge of a, what could you say about the message?

7. What would it mean to say there is an integer x equal to $\frac{1}{4}$ mod 9? If it is meaningful to say there is such an integer, what is it? Is there an integer equal to $\frac{1}{3}$ mod 9? If so, what is it?

8. By multiplying a number x times 487 in Z_{30031} we obtain 13008. If you know how to find the number x, do so. If not, explain why the problem seems difficult to do by hand.

9. Write down the addition table for $+_7$ addition. Why is the table symmetric? Why does every number appear in every row?

10. It is straightforward to solve, for x, any equation of the form

$$x +_n a = b$$

in Z_n, and to see that the result will be a unique value of x. On the other hand, we saw that 0, 3, 6, and 9 are all solutions to the equation

$$4 \cdot_{12} x = 0.$$

a) Are there any integral values of a and b, with $1 \leq a, b < 12$, for which the equation $a \cdot_{12} x = b$ does not have any solutions in Z_{12}? If there are, give one set of values for a and b. If there are not, explain how you know this.

b) Are there any integers a, with $1 < a < 12$ such that for every integral value of b, $1 \leq b < 12$, the equation $a \cdot_{12} x = b$ has a solution? If so, give one and explain why it works. If not, explain how you know this.

11. Does every equation of the form $a \cdot_n x = b$, with $a, b \in Z_n$ have a solution in Z_5? in Z_7? in Z_9? in Z_{11}?

12. Recall that if a prime number divides a product of two integers, then it divides one of the factors.

    a) Use this to show that as b runs though the integers from 0 to $p - 1$, with p prime, the products $a \cdot_p b$ are all different (for each fixed choice of a between 1 and $p - 1$).

    b) Explain why every integer greater than 0 and less than p has a unique multiplicative inverse in Z_p, if p is prime.

13. Explain why, if you were encoding messages x_1, x_2, and x_3 to obtain y_1, y_2 and y_3 by adding a mod n, your adversary would know that at least one of the differences $y_1 - y_2$, $y_1 - y_3$ or $y_2 - y_3$ taken in the integers, not in Z_n, would be the difference of two unencoded messages. (Note: we are not saying that your adversary would know which of the three was such a difference.)

14. Modular arithmetic is used in generating pseudo-random numbers. One basic algorithm (still widely used) is *linear congruential random number generation.* The following piece of code generates a sequence of numbers that may appear random to the unaware user.

```
set seed to a random value
x = seed
Repeat
        x = (ax + b) mod n
        print x
Until x = seed
```

    Execute the loop by hand for $a = 3$, $b = 7$, $n = 11$ and $seed = 0$. How "random" are these random numbers?

15. Write down the $\cdot_7$ multiplication table for Z_7.

16. Prove the equalities for multiplication in Lemma 2.3.

17. State and prove the associative law for $\cdot_n$ multiplication.

18. State and prove the distributive law for $\cdot_n$ multiplication over $+_n$ addition.

19. Write pseudocode to take m integers $x_1, x_2, \ldots, x_m$, and an integer n, and return $\Pi_i^m x_i \bmod n$. Be careful about *overflow*; in this context, being careful about overflow means that at no point should you ever compute a value that is greater than n^2.

20. Write pseudocode to decode a message that has been encoded using the algorithm

    - take three consecutive letters,
    - reverse their order,
    - interpret each as a base 26 integer (with A=0; B=1, etc.),
    - multiply that number by 37,
    - add 95 and then
    - convert that number to base 8.

    Continue this processing with each block of three consecutive letters. Append the blocks, using either an 8 or a 9 to separate the blocks. Finally, reverse the number, and replace each digit 5 by two 5's.

2.2 Inverses and GCDs

Solutions to Equations and Inverses mod n

In the last section we explored multiplication in Z_n. We saw in the special case with $n = 12$ and $a = 4$ that if we used multiplication by a in Z_n to encrypt a message, then our receiver would need to be able to solve, for x, the equation $4 \cdot_n x = b$ in order to decode a received message b. We saw that if the encrypted message was 0, then there were four possible values for x. More generally, Exercise 2.1-6 and some of the problems in the last section show that for certain values of n, a, and b, equations of the form $a \cdot_n x = b$ have a unique solution, while for other values of n, a, and b, the equation could have no solutions, or more than one solution.

To decide whether an equation of the form $a \cdot_n x = b$ has a unique solution in Z_n, it helps know whether a has a *multiplicative inverse* in Z_n, that is, whether there is another number a' such that $a' \cdot_n a = 1$. For example, in Z_9, the inverse of 2 is 5 because $2 \cdot_9 5 = 1$. On the other hand, 3 does not have an inverse in Z_9, because the equation $3 \cdot_9 x = 1$ does not have a solution. (This can be verified by checking the 9 possible values for x.) If a does have an inverse a', then we can find a solution to the equation

$$a \cdot_n x = b \ .$$

To do so, we multiply both sides of the equation by a', obtaining

$$a' \cdot_n (a \cdot_n x) = a' \cdot_n b.$$

By the associative law, this gives us

$$(a' \cdot_n a) \cdot_n x = a' \cdot_n b.$$

But $a' \cdot_n a = 1$ by definition so we have that

$$x = a' \cdot_n b \ .$$

Since this computation is valid for any x that satisfies the equation, we conclude that the only x that satisfies the equation is $a' \cdot_n b$. We summarize this discussion in the following lemma.

Lemma 2.5 *Suppose a has a multiplicative inverse a' in Z_n. Then for any $b \in Z_n$, the equation*

$$a \cdot_n x = b$$

has the unique solution

$$x = a' \cdot_n b \ .$$

Note that this lemma holds for *any* value of $b \in Z_n$.

This lemma tells us that whether or not a number has an inverse mod n is important for the solution of modular equations. We therefore wish to understand exactly when a member of Z_n has an inverse.

Inverses mod n

We will consider some of the examples related to Problem 11 of the last section.

Exercise 2.2-1 Determine whether every element a of Z_n has an inverse for n= 5, 6, 7, 8, and 9.

Exercise 2.2-2 If an element of Z_n has a multiplicative inverse, can it have two different multiplicative inverses?

For Z_5, we can determine by multiplying each pair of nonzero members of Z_5 that the following table gives multiplicative inverses for each element a of Z_5. For example, the products $2 \cdot_5 1 = 2$, $2 \cdot_5 2 = 4$, $2 \cdot_5 3 = 1$, and $2 \cdot_5 4 = 3$ tell us that 3 is the unique multiplicative inverse for 2 in Z_5. This is the reason we put 3 below 2 in the table. One can make the same kinds of computations with 3 or 4 instead of 2 on the left side of the products to get the rest of the table.

a	1	2	3	4
a'	1	3	2	4

For Z_7, we have similarly the table

a	1	2	3	4	5	6
a'	1	4	5	2	3	6

.

For Z_9, we have already said that $3 \cdot_9 x = 1$ does not have a solution, so by Lemma 2.5, 3 does not have an inverse. (Notice how we are using the Lemma. The Lemma says that if 3 had an inverse, then the equation $3 \cdot_9 x = 1$ *would* have a solution, and this would contradict the fact that $3 \cdot_9 x = 1$ does not have a solution. Thus assuming that 3 had an inverse would lead us to a contradiction. Therefore 3 has no multiplicative inverse.)

This computation is a special case of the following corollary[4] to Lemma 2.5.

Corollary 2.6 *Suppose there is a b in Z_n such that the equation*

$$a \cdot_n x = b$$

does not have a solution. Then a does not have a multiplicative inverse in Z_n.

Proof: Suppose that $a \cdot_n x = b$ has no solution. Suppose further that a does have a multiplicative inverse a' in Z_n. Then by Lemma 2.5, $x = a'b$ is a solution to the equation $a \cdot_n x = b$. This contradicts the hypothesis given in the corollary that the equation does not have a solution. Thus some supposition we made above must be incorrect. One of the assumptions, namely that $a \cdot_n x = b$ has no solution was the hypothesis given to us in the statement of the corollary. The only other supposition we made was that a has an inverse a' in Z_n. Thus this supposition must be incorrect as it led to the contradiction. Therefore, it must be case that a does not have a multiplicative inverse in Z_n. ■

Our proof of the corollary is a classical example of the use of contradiction in a proof. The principle of *proof by contradiction* is the following.

[4]In the next section we shall see that this corollary is actually equivalent to Lemma to Lemma 2.5.

Principle 2.1 (Proof by contradiction) *If by assuming a statement we want to prove is false, we are lead to a contradiction, then the statement we are trying to prove must be true.*

We can actually give more information than Exercise 1 asks for. You can check that the table below shows an X for the elements of Z_9 that do not have inverses and gives an inverse for each element that has one

a	1	2	3	4	5	6	7	8
a'	1	5	X	7	2	X	4	8

In Z_6, 1 has an inverse, namely 1, but the equations

$$2 \cdot_6 1 = 2, \quad 2 \cdot_6 2 = 4, \quad 2 \cdot_6 3 = 0, \quad 2 \cdot_6 4 = 2, \quad 2 \cdot_6 5 = 4$$

tell us that 2 does not have an inverse. Less directly, but with less work, we see that the equation $2 \cdot_6 x = 3$ has no solution because $2x$ will always be even, so $2x$ mod 6 will always be even. Then Corollary 2.6 tells us that 2 has no inverse. Once again, we give a table that shows exactly which elements of Z_6 have inverses.

a	1	2	3	4	5
a'	1	X	X	X	5

A similar set of equations shows that 2 does not have an inverse in Z_8. The following table shows which elements of Z_8 have inverses.

a	1	2	3	4	5	6	7
a'	1	X	3	X	5	X	7

We see that every nonzero element in Z_5 and Z_7 does have a multiplicative inverse, but in Z_6, Z_8, and Z_9, some elements do not have a multiplicative inverse. Notice that 5 and 7 are prime, while 6, 8, and 9 are not. Further notice that the elements in Z_n that do not have a multiplicative inverse are exactly those that share a common factor with n.

We showed that 2 has exactly one inverse in Z_5 by checking each multiple of 2 in Z_5 and showing that exactly one multiple of 2 equals 1. In fact, for any element that has an inverse in Z_5, Z_6, Z_7, Z_8, and Z_9, you can check in the same way that it has exactly one inverse. We explain why in a theorem.

Theorem 2.7 *If an element of Z_n has a multiplicative inverse, then it has exactly one inverse.*

Proof: Suppose that an element a of Z_n has an inverse a'. Suppose that a^* is also an inverse of a. Then a' is a solution to $a \cdot_n x = 1$ and a^* is a solution to $a \cdot_n x = 1$. But by Lemma 2.5, the equation $a \cdot_n x = 1$ has a unique solution. Therefore $a' = a^*$. ■

Just as we use a^{-1} to denote the inverse of a in the real numbers, we use a^{-1} to denote the unique inverse of a in Z_n when a has an inverse. Now we can say precisely what we mean by division in Z_n. We will define what we mean by *dividing* a member of Z_n by a only in the case that a has an inverse a^{-1} mod n. In this case dividing b by a mod n is defined to be same as multiplying b by a^{-1} mod n. We were led to our discussion of inverses because of their role in solving equations. We observed that in our examples, an element of Z_n that has an inverse mod n has no factors greater than 1 in common with n. This is a statement about a and n as integers with ordinary multiplication rather than multiplication mod n. Thus to prove that a has an inverse mod n if and only if a and n have no common factors other than 1 and -1, we have to convert the equation $a \cdot_n x = 1$ into an equation involving ordinary multiplication.

Converting Modular Equations to Normal Equations

We can re-express the equation

$$a \cdot_n x = 1$$

as

$$ax \bmod n = 1.$$

But the definition of $ax \bmod n$ is that it is the remainder r we get when we write $ax = qn+r$, with $0 \leq r < n$. This means that $ax \bmod n = 1$ if and only if there is an integer q with $ax = qn + 1$, or

$$ax - qn = 1. \tag{2.8}$$

Thus we have shown

Lemma 2.8 *The equation*

$$a \cdot_n x = 1$$

has a solution in Z_n if and only if there exist integers x and y such that

$$ax + ny = 1.$$

Proof: We simply take $y = -q$. ■

We make the change from $-q$ to y for two reasons. First, if you read a number theory book, you are more likely to see the equation with y in this context. Second, to solve this equation, we must find both x and y, and so using a letter near the end of the alphabet in place of $-q$ emphasizes that this is a variable for which we need to solve.

It appears that we have made our work harder, not easier, as we have converted the problem of solving (in Z_n) the equation $a \cdot_n x = 1$, an equation with just one variable x (that could only have $n-1$ different values), to a problem of solving Equation 2.8, which has two variables, x and y. Further, in this second equation, x and y can take on any integer values, even negative values.

However, this equation will prove to be exactly what we need to prove that a has an inverse mod n if and only if a and n have no common factors larger than one.

Greatest Common Divisors (GCD)

Exercise 2.2-3 Suppose that a and n are integers such that $ax+ny = 1$, for some integers x and y. What does that tell us about being able to find a (multiplicative) inverse for a (mod n)? In this situation, if a has an inverse in Z_n, what is it?

Exercise 2.2-4 If $ax+ny = 1$ for integers x and y, can a and n have any common divisors other than 1 and -1?

In Exercise 2.2-3, since by Lemma 2.8, the equation $a \cdot_n x = 1$ has a solution in Z_n if and only if there exist integers x and y such that $ax + ny = 1$, we can can conclude that

Theorem 2.9 *A number a has a multiplicative inverse in Z_n if and only if there are integers x and y such that $ax + ny = 1$.*

We answer the rest of Exercise 2.2-3 with a corollary.

Corollary 2.10 *If $a \in Z_n$ and x and y are integers such that $ax+ny = 1$, then the multiplicative inverse of a in Z_n is $x \bmod n$.*

Proof: Since $n \cdot_n y = 0$ in Z_n, we have $a \cdot_n x = 1$ in Z_n and therefore x is the inverse of a in Z_n. ■

Now let's consider Exercise 2.2-4. If a and n have a common divisor k, then there must exist integers s and q such that

$$a = sk$$

and

$$n = qk\ .$$

Substituting these into $ax + ny = 1$, we obtain

$$\begin{aligned} 1 &= ax + ny \\ &= skx + qky \\ &= k(sx + qy). \end{aligned}$$

But then k is a divisor of 1. Since the only integer divisors of 1 are ± 1, we must have $k = \pm 1$. Therefore a and n can have no common divisors other than 1 and -1.

In general, the **greatest common divisor** of two numbers j and k is the largest number d that is a factor of both j and k.[5] We denote the greatest common divisor of j and k by $\gcd(j, k)$.

We can now restate Exercise 2.2-4 as follows:

Lemma 2.11 *Given a and n, if there exist integers x and y such that $ax + ny = 1$ then $\gcd(a, n) = 1$.*

If we combine Theorem 2.9 and Lemma 2.11, we see that that if a has a multiplicative inverse mod n, then $\gcd(a, n) = 1$. It is natural to ask whether the statement that "if $\gcd a, n = 1$, then a has a multiplicative inverse" is true as well.[6] If so, this would give us a way to test whether a has a multiplicative inverse mod n by computing the greatest common divisor of a and n. For this purpose we would need an algorithm to find $\gcd(a, n)$. It turns out that there is such an algorithm, and a byproduct of the algorithm is a proof of our conjectured converse statement! When two integers j and k have $\gcd(j, k) = 1$, we say that j and k are *relatively prime*.

Euclid's Division Theorem

One of the important tools in understanding greatest common divisors is Euclid's Division Theorem, a result which has already been important to us in defining what we mean by $m \bmod n$. While it appears obvious, as do some other theorems in number theory, it follows from simpler principles of number theory, and the proof helps us understand how the greatest common divisor

[5] There is one common factor of j and k for sure, namely 1. No common factor can be larger than the smaller of j and k in absolute value, and so there must be a largest common factor.

[6] Notice that this statement is *not* equivalent to the statement in the lemma. This statement is what is called the "converse" of the lemma; we will explain the idea of converse statements more in Chapter 3.

algorithm works. Thus we restate it and present a proof here. Our proof uses the method of proof by contradiction, which you first saw in Corollary 2.6. Notice that we are assuming m is nonnegative which we didn't assume in our earlier statement of Euclid's Division Theorem, Theorem 2.1. In Problem 16 we will explore how we can remove this additional assumption.

Theorem 2.12 (Euclid's Division Theorem, restricted version) *For every nonnegative integer m and positive integer n, there exist unique integers q and r such that $m = nq + r$ and $0 \le r < n$. By definition, r is equal to $m \bmod n$.*

Proof: To prove this theorem, assume instead, for purposes of contradiction, that it is false. Among all pairs (m, n) that make it false, choose the smallest m that makes it false. We cannot have $m < n$ because then the statement would be true with $q = 0$ and $r = m$, and we cannot have $m = n$ because then the statement is true with $q = 1$ and $r = 0$. This means $m - n$ is a positive number smaller than m. We assumed that m was the smallest value that made the theorem false, and so the theorem must be true for the pair $(m - n, n)$. Therefore, there must exist a q' and r' such that

$$m - n = q'n + r', \text{ with } 0 \le r' < n.$$

Thus $m = (q'+1)n + r'$. Now, by setting $q = q' + 1$ and $r = r'$, we can satisfy the theorem for the pair (m, n), contradicting the assumption that the statement is false. Thus the only possibility is that the statement is true. ■

The proof technique used here is a special case of proof by contradiction. We call the technique *proof by smallest counterexample*. In this method, we assume, as in all proofs by contradiction, that the theorem is false. This implies that there must be a *counterexample* which does not satisfy the conditions of the theorem. In this case that counterexample would consist of numbers m and n such that *no* integers q and r exist which satisfy $m = qn + r$. Further, if there are counterexamples, then there must be one having the smallest m. We assume we have chosen a counter example with such a smallest m. the we reason that if such an m exists, then every example wit a smaller m satisfies the conclusion of the theorem. If we can then use a smaller true example to show that our supposedly false example is true as well, we have created a contradiction. The only thing this can contradict is our assumption that the theorem was false. Therefore this assumption has to be invalid, and the theorem has to be true. As we will see in Chapter 4.1, this method is closely related to a proof method called *proof by induction* and to recursive algorithms. In essence, the proof of Theorem 2.1 describes a recursive program to find q and r in the theorem above so that $0 \le r < n$.

Exercise 2.2-5 Suppose that $k = jq + r$ as in Euclid's Division Theorem. Is there a relationship between $\gcd(j, k)$ and $\gcd(r, j)$?

In this exercise, if $r = 0$, then $\gcd(r, j)$ is j, because any number is a divisor of zero. But this is the GCD of k and j as well since in this case $k = jq$. The answer to the remainder of Exercise 2.2-5 appears in the following lemma.

Lemma 2.13 *If j, k, q, and r are positive integers such that $k = jq + r$ then*

$$\gcd(j, k) = \gcd(r, j). \tag{2.9}$$

Proof: In order to prove that both sides of Equation 2.9 are equal, we will show that they have exactly the same set of factors. That is, we will first show that if d is a factor of the left-hand side, then it is a factor of the right-hand side. Second, we will show that if d is a factor of the right-hand side, then it is a factor of the left-hand side.

If d is a factor of $\gcd(j,k)$ then it is a factor of both j and k. There must be integers i_1 and i_2 so that $k = i_1 d$ and $j = i_2 d$. Thus d is also a factor of

$$\begin{aligned} r &= k - jq \\ &= i_1 d - i_2 dq \\ &= (i_1 - i_2 q)d \ . \end{aligned}$$

Since d is a factor of j (by supposition) and r (by the equation above), it must be a factor of $\gcd(r,j)$.

Similarly, if d is a factor of $\gcd(r,j)$, it is a factor of j and r, and we can write $j = i_3 d$ and $r = i_4 d$. Therefore,

$$\begin{aligned} k &= jq + r \\ &= i_3 dq + i_4 d \\ &= (i_3 q + i_4)d \ , \end{aligned}$$

and d is a factor of k and therefore of $\gcd(j,k)$.

Since $\gcd(j,k)$ has the same factors as $\gcd(r,j)$ they must be equal. ■

While we did not need to assume $r < j$ in order to prove the lemma, Theorem 2.1 tells us we may assume $r < j$. The assumption in the lemma that j, q and r are positive implies that $j < k$. Thus this lemma reduces our problem of finding $\gcd(j,k)$ to the simpler (in a recursive sense) problem of finding $\gcd(r,j)$.

The GCD Algorithm

Exercise 2.2-6 Using Lemma 2.13, write a recursive algorithm to find $\gcd(j,k)$, given that $j \le k$. Use it (by hand) to find the GCD of 24 and 14 and the GCD of 252 and 189.

Our algorithm for Exercise 2.2-6 is based on Lemma 2.13 and the observation that if $k = jq$, for any q, then $j = \gcd(j,k)$. We first write $k = jq + r$ in the usual way. If $r = 0$, then we return j as the greatest common divisor. Otherwise, we apply our algorithm to find the greatest common divisor of j and r. Finally, we return the result as the greatest common divisor of j and k.

To find

$$\gcd(14, 24)$$

we write

$$24 = 14(1) + 10.$$

In this case $k = 24$, $j = 14$, $q = 1$ and $r = 10$. Thus we can apply Lemma 2.13 and conclude that

$$\gcd(14, 24) = \gcd(10, 14).$$

We therefore continue our computation of $\gcd(10,14)$, by writing $14 = 10 \cdot 1 + 4$, and have that

$$\gcd(10,14) = \gcd(4,10).$$

Now,

$$10 = 4 \cdot 2 + 2,$$

and so

$$\gcd(4,10) = \gcd(2,4).$$

Now

$$4 = 2 \cdot 2 + 0,$$

so that now $k = 4$, $j = 2$, $q = 2$, and $r = 0$. In this case our algorithm tells us that our current value of j is the GCD of the original j and k. This step is the base case of our recursive algorithm. Thus we have that

$$\gcd(14,24) = \gcd(2,4) = 2.$$

While the numbers are larger, it turns out to be even easier to find the GCD of 252 and 189. We write

$$252 = 189 \cdot 1 + 63,$$

so that $\gcd(189,252) = \gcd(63,189)$, and

$$189 = 63 \cdot 3 + 0.$$

This tells us that $\gcd(189,252) = \gcd(189,63) = 63$.

Extended GCD algorithm

By analyzing our process in a bit more detail, we will be able to return not only the greatest common divisor, but also numbers x and y such that $\gcd(j,k) = jx + ky$. This will solve the problem we have been working on, because it will prove that if $\gcd(a,n) = 1$, then there are integers x and y such that $ax + ny = 1$. Further it will tell us how to find x, and therefore the multiplicative inverse of a.

In the case that $k = jq$ and we want to return j as our greatest common divisor, we also want to return 1 for the value of x and 0 for the value of y. Suppose we are now in the case that that $k = jq + r$ with $0 < r < j$ (that is, the case that $k \neq jq$). Then we recursively compute $\gcd(r,j)$ and in the process get an x' and a y' such that $\gcd(r,j) = rx' + jy'$. Since $r = k - jq$, we get by substitution that

$$\gcd(r,j) = (k - jq)x' + jy' = kx' + j(y' - qx').$$

Thus when we return $\gcd(r,j)$ as $\gcd(j,k)$, we want to return the value of x' as y and and the value of $y' - qx'$ as x.

We will refer to the process we just described as "Euclid's extended GCD algorithm."

Exercise 2.2-7 Apply Euclid's extended GCD algorithm to find numbers x and y such that the GCD of 14 and 24 is $14x + 24y$.

For our discussion of Exercise 2.2-7 we give pseudocode for the extended GCD algorithm. While we expressed the algorithm more concisely earlier by using recursion, we will give an iterative version that is longer but can make the computational process clearer. Instead of using the variables q, j, k, r, x and y, we will use six arrays, where $q[i]$ is the value of q computed on the ith iteration, and so forth. We will use the index zero for the input values, that is $j[0]$ and $k[0]$ will be the numbers whose gcd we wish to compute. Eventually $x[0]$ and $y[0]$ will become the x and y we want.

(In Line 0 we are using the notation $\lfloor x \rfloor$ to stand for the floor of x, the largest integer less than or equal to x.)

<u>gcd(j, k)</u>

`// assume that` $j < k$
(1) $i = 0; k[i] = k; j[i] = j$
(2) `Repeat`
(3) $\quad q[i] = \lfloor k[i]/j[i] \rfloor$
(4) $\quad r[i] = k[i] - q[i]j[i]$
(5) $\quad k[i+1] = j[i]; j[i+1] = r[i]$
(6) $\quad i = i + 1$
(7) `Until` $(r[i-1] = 0)$
`// we have found the value of the gcd, now we compute the` x `and` y
(8) $i = i - 1$
(9) $gcd = j[i]$
(10) $y[i] = 0; x[i] = 1$
(11) $i = i - 1$
(12) `While` $(i \geq 0)$
(13) $\quad y[i] = x[i+1]$
(14) $\quad x[i] = y[i+1] - q[i]x[i+1]$
(15) $\quad i = i - 1$
(16) `Return` gcd
(17) `Return` x
(18) `Return` y

We show the details of how this algorithm applies to gcd$(24, 14)$ in Table 2.1. In a row, the $q[i]$ and $r[i]$ values are computed from the $j[i]$ and $k[i]$ values. Then the $j[i]$ and $r[i]$ are passed down to the next row as $k[i+1]$ and $j[i+1]$ respectively. This process continues until we finally reach a case where $k[i] = q[i]j[i]$ and we can answer $j[i]$ for the gcd. We can then begin computing $x[i]$ and $y[i]$. In the row with $i = 3$, we have that $x[i] = 0$ and $y[i] = 1$. Then, as i decreases, we compute $x[i]$ and $y[i]$ for a row by setting $y[i]$ to $x[i+1]$ and $x[i]$ to $y[i+1] - q[i]x[i+1]$. We note that in every row, we have the property that $j[i]x[i] + k[i]y[i] = \gcd(j, k)$.

We summarize Euclid's extended GCD algorithm in the following theorem:

Theorem 2.14 *Given two integers j and k, Euclid's extended GCD algorithm computes* $\gcd(j, k)$ *and two integers x and y such that* $\gcd(j, k) = jx + ky$.

We now use Eculid's extended GCD algorithm to extend Lemma 2.11.

i	$j[i]$	$k[i]$	$q[i]$	$r[i]$	$x[i]$	$y[i]$
0	14	24	1	10		
1	10	14	1	4		
2	4	10	2	2		
3	2	4	2	0	1	0
2	4	10	2	2	-2	1
1	10	14	1	4	3	-2
0	14	24	1	10	-5	3
gcd = 2						
$x = -5$						
$y = 3$						

Table 2.1: The computation of gcd(14, 24) by algorithm gcd(j, k).

Theorem 2.15 *Two positive integers j and k have greatest common divisor 1 (and thus are relatively prime) if and only if there are integers x and y such that $jx + ky$=1.*

Proof: The statement that if there are integers x and y such that $jx+ky = 1$, then $\gcd(j, k) = 1$ is proved in Lemma 2.11. In other words, $\gcd(j, k) = 1$ if there are integers x and y such that $jx + ky = 1$.

On the other hand, we just showed, by Euclid's extended GCD algorithm, that given positive integers j and k, there are integers x and y such that $\gcd(j, k) = jx+ky$. Therefore, $\gcd(j, k) = 1$ only if there are integers x and y such that $jx + ky = 1$. ■

Combining Lemma 2.8 and Theorem 2.15, we obtain:

Corollary 2.16 *For any positive integer n, an element a of Z_n has a multiplicative inverse if and only if* $\gcd(a, n) = 1$.

Using the fact that if n is prime, $\gcd(a, n) = 1$ for all non-zero $a \in Z_n$, we obtain

Corollary 2.17 *For any prime p, every non-zero element a of Z_p has an inverse.*

Computing Inverses

Not only does Euclid's extended GCD algorithm tell us if an inverse exists, but, just as we saw in Exercise 2.2-3 it computes it for us. Combining Exercise 2.2-3 with Theorem 2.15, we get

Corollary 2.18 *If an element a of Z_n has an inverse, we can compute it by running Euclid's extended GCD algorithm to determine integers x and y so that $ax + ny = 1$. Then the inverse of a in Z_n is $x \bmod n$.*

For completeness, we now give pseudocode which determines whether an element a in Z_n has an inverse and computes the inverse if it exists:

```
inverse(a, n)
(1)  Run procedure gcd(a, n) to obtain gcd(a, n), x and y
(2)  if gcd(a, n) = 1
(3)       return x
(4)  else
(5)       print ‘‘no inverse exists’’
```

The correctness of the algorithm follows immediately from the fact that $\gcd(a,n) = ax + ny$, so if $\gcd(a,n) = 1$, $ax \bmod n$ must be equal to 1.

Important Concepts, Formulas, and Theorems

1. *Multiplicative inverse.* a' is a multiplicative inverse of a in Z_n if $a \cdot_n a' = 1$. If a has a multiplicative inverse, then it has a unique multiplicative inverse which we denote by a^{-1}.

2. *An important way to solve modular equations.* Suppose a has a multiplicative inverse mod n, and this inverse is a^{-1}. Then for any $b \in Z_n$, the unique solution to the equation
$$a \cdot_n x = b$$
is
$$x = a^{-1} \cdot_n b\ .$$

3. *Converting modular to regular equations.* The equation
$$a \cdot_n x = 1$$
has a solution in Z_n if and only if there exist integers x and y such that
$$ax + ny = 1\ .$$

4. *When do inverses exist in Z_n?* A number a has a multiplicative inverse in Z_n if and only if there are integers x and y such that $ax + ny = 1$.

5. *Greatest common divisor (GCD).* The *greatest common divisor* of two numbers j and k is the largest number d that is a factor of both j and k.

6. *Relatively prime.* When two numbers, j and k have $\gcd(j,k) = 1$, we say that j and k are relatively prime.

7. *Connecting inverses to GCD.* Given a and n, if there exist integers x and y such that $ax + ny = 1$ then $\gcd(a,n) = 1$.

8. *GCD recursion lemma.* If j, k, q, and r are positive integers such that $k = jq + r$ then $\gcd(j,k) = \gcd(r,j)$.

9. *Euclid's GCD algorithm.* Given two numbers j and k, this algorithm returns $\gcd(j,k)$.

10. *Euclid's extended GCD algorithm.* Given two numbers j and k, this algorithm returns $\gcd(j,k)$, and two integers x and y such that $\gcd(j,k) = jx + ky$.

11. *Relating GCD of 1 to Euclid's extended GCD algorithm.* Two positive integers j and k have greatest common divisor 1 if and only if there are integers x and y such that $jx + ky$=1. One of the integers x and y could be negative.

12. *Restatement for Z_n.* $\gcd(a, n) = 1$ if and only if there are integers x and y such that $ax + ny = 1$.

13. *Condition for multiplicative inverse in Z_n* For any positive integer n, an element a of Z_n has an inverse if and only if $\gcd(a, n) = 1$.

14. *Multiplicative inverses in Z_p, p prime* For any prime p, every non-zero element a of Z_p has a multiplicative inverse.

15. *A way to solve some modular equations $a \cdot_n x = b$.* Use Euclid's extended GCD algorithm to compute a^{-1} (if it exists), and multiply both sides of the equation by a^{-1}. (If a has no inverse, the equation might or might not have a solution.)

Problems

1. If $a \cdot 133 - m \cdot 277 = 1$, does this guarantee that a has an inverse mod m? If so, what is it? If not, why not?

2. If $a \cdot 133 - 2m \cdot 277 = 1$, does this guarantee that a has an inverse mod m? If so, what is it? If not, why not?

3. Determine whether every nonzero element of Z_n has a multiplicative inverse for $n = 10$ and $n = 11$.

4. How many elements a are there such that $a \cdot_{31} 22 = 1$? How many elements a are there such that $a \cdot_{10} 2 = 1$?

5. Given an element b in Z_n, what can you say in general about the possible number of elements a such that $a \cdot_n b = 1$ in Z_n?

6. If $a \cdot 133 - m \cdot 277 = 1$, what can you say about all possible common divisors of a and m?

7. Compute the GCD of 210 and 126 by using Euclid's GCD algorithm.

8. If $k = jq + r$ as in Euclid's Division Theorem, is there a relationship between $\gcd(q, k)$ and $\gcd(r, q)$. If so, what is it?

9. Bob and Alice want to choose a key they can use for cryptography, but all they have to communicate is a bugged phone line. Bob proposes that they each choose a secret number, a for Alice and b for Bob. They also choose, over the phone, a prime number p with more digits than any key they want to use, and one more number q. Bob will send Alice bq mod p, and Alice will send Bob aq mod p. Their key (which they will keep secret) will then be abq mod p. (Here we don't worry about the details of how they use their key, only with how they choose it.) As Bob explains, their wire tapper will know p, q, aq mod p, and bq mod p, but will not know a or b, so their key should be safe.

   Is this scheme safe, that is can the wiretapper compute abq mod p? If so, how does she do it?

Alice says "You know, the scheme sounds good, but wouldn't it be more complicated for the wire tapper if I send you $q^a \bmod p$, you send me $q^b \pmod p$ and we use $q^{ab} \bmod p$ as our key?" In this case can you think of a way for the wire tapper to compute $q^{ab} \bmod p$? If so, how can you do it? If not, what is the stumbling block? (It is fine for the stumbling block to be that you don't know how to compute something; you don't need to prove that you can't compute it.)

10. Write pseudocode for a recursive version of the extended GCD algorithm.

11. Run Euclid's extended GCD algorithm to compute $\gcd(576, 486)$. Show all the steps.

12. Use Euclid's extended GCD algorithm to compute the multiplicative inverse of 16 modulo 103.

13. Solve the equation $16 \cdot_{103} x = 21$ in Z_{103}.

14. Which elements of Z_{35} do not have multiplicative inverses in Z_{35}?

15. If $k = jq + r$ as in Euclid's Division Theorem, is there a relationship between $\gcd(j, k)$ and $\gcd(r, k)$. If so, what is it?

16. Notice that if m is negative, then $-m$ is positive, so that by Theorem 2.12 $-m = qn + r$, where $0 \le r < n$. This gives us $m = -qn - r$. If $r = 0$, then we have written $m = q'n + r'$, where $0 \le r' \le n$ and $q' = -q$. However if $r > 0$, we cannot take $r' = -r$ and have $0 \le r' < n$. Notice, though, that since since we have already finished the case $r = 0$ we may assume that $0 \le n - r < n$. This suggests that if we were to take r' to be $n - r$, we might be able to find a q' so that $m = q'n + r'$ with $0 \le r' \le n$, which would let us conclude that Euclid's Division Theorem is valid for negative values m as well as nonnegative values m. Find a q' that works and explain how you have extended Euclid's Division Theorem from the version in Theorem 2.12 to the version in Theorem 2.1.

17. The Fibonacci numbers F_i are defined as follows:

$$F_i = \begin{cases} 1 & \text{if } i \text{ is 1 or 2} \\ F_{i-1} + F_{i-2} & \text{otherwise.} \end{cases}$$

    What happens when you run Euclid's extended GCD algorithm on F_i and F_{i-1}? (We are asking about the execution of the algorithm, not just the answer.)

18. Write (and run on several different inputs) a program to implement Euclid's extended GCD algorithm. Be sure to return x and y in addition to the GCD. About how many times does your program have to make a recursive call to itself? What does that say about how long we should expect it to run as we increase the size of the j and k whose GCD we are computing?

19. The least common multiple of two positive integers x and y is the smallest positive integer z such that z is an integer multiple of both x and y. Give a formula for the least common multiple that involves the GCD.

20. Write pseudocode that given integers a, b and n in Z_n, either computes an x such that $a \cdot_n x = b$ or concludes that no such x exists.

21. Give an example of an equation of the form $a \cdot_n x = b$ that has a solution even though a and n are not relatively prime, or show that no such equation exists.

22. Either find an equation of the form $a \cdot_n x = b$ in Z_n that has a unique solution even though a and n are not relatively prime, or prove that no such equation exists. In other words, you are either to prove the statement that if $a \cdot_n x = b$ has a unique solution in Z_n, then a and n are relatively prime or to find a counter example.

2.3 The RSA Cryptosystem

Exponentiation mod n

In the previous sections, we have considered encryption using modular addition and multiplication, and have seen the shortcomings of both. In this section, we will consider using exponentiation for encryption, and will show that it provides a much greater level of security.

The idea behind RSA encryption is *exponentiation* in Z_n. By Lemma 2.3, if $a \in Z_n$,

$$a^j \bmod n = \underbrace{a \cdot_n a \cdot_n \cdots \cdot_n a}_{j \text{ factors}}. \tag{2.10}$$

In other words $a^j \bmod n$ is the product in Z_n of j factors, each equal to a.

The Rules of Exponents

Lemma 2.3 and the rules of exponents for the integers tell us that

Lemma 2.19 *For any $a \in Z_n$, and any nonnegative integers i and j,*

$$(a^i \bmod n) \cdot_n (a^j \bmod n) = a^{i+j} \bmod n \tag{2.11}$$

and

$$(a^i \bmod n)^j \bmod n = a^{ij} \bmod n. \tag{2.12}$$

Exercise 2.3-1 Compute the powers of 2 mod 7. What do you observe? Now compute the powers of 3 mod 7. What do you observe?

Exercise 2.3-2 Compute the sixth powers of the nonzero elements of Z_7. What do you observe?

Exercise 2.3-3 Compute the numbers $1 \cdot_7 2$, $2 \cdot_7 2$, $3 \cdot_7 2$, $4 \cdot_7 2$, $5 \cdot_7 2$, and $6 \cdot_7 2$. What do you observe? Now compute the numbers $1 \cdot_7 3$, $2 \cdot_7 3$, $3 \cdot_7 3$, $4 \cdot_7 3$, $5 \cdot_7 3$, and $6 \cdot_7 3$. What do you observe?

Exercise 2.3-4 Suppose we choose an arbitrary nonzero number a between 1 and 6. Are the numbers $1 \cdot_7 a$, $2 \cdot_7 a$, $3 \cdot_7 a$, $4 \cdot_7 a$, $5 \cdot_7 a$, and $6 \cdot_7 a$ all different? Why or why not?

In Exercise 2.3-1, we have that

$$\begin{aligned}
2^0 \bmod 7 &= 1\\
2^1 \bmod 7 &= 2\\
2^2 \bmod 7 &= 4\\
2^3 \bmod 7 &= 1\\
2^4 \bmod 7 &= 2\\
2^5 \bmod 7 &= 4\\
2^6 \bmod 7 &= 1\\
2^7 \bmod 7 &= 2\\
2^8 \bmod 7 &= 4.
\end{aligned}$$

Continuing, we see that the powers of 2 will cycle through the list of three values $1, 2, 4$ again and again. Performing the same computation for 3, we have

$$\begin{aligned}
3^0 \bmod 7 &= 1\\
3^1 \bmod 7 &= 3\\
3^2 \bmod 7 &= 2\\
3^3 \bmod 7 &= 6\\
3^4 \bmod 7 &= 4\\
3^5 \bmod 7 &= 5\\
3^6 \bmod 7 &= 1\\
3^7 \bmod 7 &= 3\\
3^8 \bmod 7 &= 2.
\end{aligned}$$

In this case, we will cycle through the list of six values $1, 3, 2, 6, 4, 5$ again and again.

Now observe that in Z_7, $2^6 = 1$ and $3^6 = 1$. This suggests an answer to Exercise 2.3-2. Is it the case that $a^6 \bmod 7 = 1$ for all $a \in Z_7$? We can compute that $1^6 \bmod 7 = 1$, and

$$\begin{aligned}
4^6 \bmod 7 &= (2 \cdot_7 2)^6 \bmod 7\\
&= (2^6 \cdot_7 2^6) \bmod 7\\
&= (1 \cdot_7 1) \bmod 7\\
&= 1.
\end{aligned}$$

What about 5^6? Notice that $3^5 = 5$ in Z_7 by the computations we made above. Using Equation 2.12 twice, this gives us

$$\begin{aligned}
5^6 \bmod 7 &= (3^5)^6 \bmod 7\\
&= 3^{5\cdot 6} \bmod 7\\
&= 3^{6\cdot 5} \bmod 7\\
&= (3^6)^5 = 1^5 = 1
\end{aligned}$$

in Z_7. Finally, since $-1 \bmod 7 = 6$, Lemma 2.3 tells us that $6^6 \bmod 7 = (-1)^6 \bmod 7 = 1$. Thus the sixth power of each element of Z_7 is 1.

In Exercise 2.3-3 we see that

$$\begin{aligned}
1 \cdot_7 2 &= 1 \cdot 2 \bmod 7 = 2\\
2 \cdot_7 2 &= 2 \cdot 2 \bmod 7 = 4\\
3 \cdot_7 2 &= 3 \cdot 2 \bmod 7 = 6\\
4 \cdot_7 2 &= 4 \cdot 2 \bmod 7 = 1\\
5 \cdot_7 2 &= 5 \cdot 2 \bmod 7 = 3\\
6 \cdot_7 2 &= 6 \cdot 2 \bmod 7 = 5.
\end{aligned}$$

Thus these numbers are a permutation of the set $\{1, 2, 3, 4, 5, 6\}$. Similarly,

$$\begin{aligned}
1 \cdot_7 3 &= 1 \cdot 3 \bmod 7 = 3\\
2 \cdot_7 3 &= 2 \cdot 3 \bmod 7 = 6
\end{aligned}$$

$$\begin{array}{rcccl} 3 \cdot_7 3 &=& 3 \cdot 3 \bmod 7 &=& 2 \\ 4 \cdot_7 3 &=& 4 \cdot 3 \bmod 7 &=& 5 \\ 5 \cdot_7 3 &=& 5 \cdot 3 \bmod 7 &=& 1 \\ 6 \cdot_7 3 &=& 6 \cdot 3 \bmod 7 &=& 4. \end{array}$$

Again we get a permutation of $\{1, 2, 3, 4, 5, 6\}$.

In Exercise 2.3-4 we are asked whether this is always the case. Notice that since 7 is a prime, by Corollary 2.17, each nonzero number between 1 and 6 has a mod 7 multiplicative inverse a^{-1}. Thus if i and j were integers in Z_7 with $i \cdot_7 a = j \cdot_7 a$, we multiply mod 7 on the right by a^{-1} to get

$$(i \cdot_7 a) \cdot_7 a^{-1} = (j \cdot_7 a) \cdot_7 a^{-1}.$$

After using the associative law we get

$$i \cdot_7 (a \cdot_7 a^{-1}) = j \cdot_7 (a \cdot_7 a^{-1}). \tag{2.13}$$

Since $a \cdot_7 a^{-1} = 1$, Equation 2.13 simply becomes $i = j$. Thus, we have shown that the only way for $i \cdot_7 a$ to equal $j \cdot_7 a$ is for i to equal j. Therefore, all the values $i \cdot_7 a$ for $i = 1, 2, 3, 4, 5, 6$ must be different. Since we have six different values, all between 1 and 6, we have that the values ia for $i = 1, 2, 3, 4, 5, 6$ are a permutation of $\{1, 2, 3, 4, 5, 6\}$.

As you can see, the only fact we used in our analysis of Exercise 2.3-4 is that if p is a prime, then any number between 1 and $p-1$ has a multiplicative inverse in Z_p. In other words, we have really proved the following lemma.

Lemma 2.20 *Let p be a prime number. For any fixed nonzero number a in Z_p, the numbers $(1 \cdot a) \bmod p$, $(2 \cdot a) \bmod p$, …, $((p-1) \cdot a) \bmod p$, are a permutation of the set $\{1, 2, \cdots, p-1\}$.*

With this lemma in hand, we can prove a famous theorem that explains the phenomenon we saw in Exercise 2.3-2.

Fermat's Little Theorem

Theorem 2.21 *(Fermat's Little Theorem). Let p be a prime number. Then $a^{p-1} \bmod p = 1$ in Z_p for each nonzero a in Z_p.*

Proof: Since p is a prime, Lemma 2.20 tells us that the numbers $1 \cdot_p a$, $2 \cdot_p a$, …, $(p-1) \cdot_p a$, are a permutation of the set $\{1, 2, \cdots, p-1\}$. But then

$$1 \cdot_p 2 \cdot_p \cdots \cdot_p (p-1) = (1 \cdot_p a) \cdot_p (2 \cdot_p a) \cdot_p \cdots \cdot_p ((p-1) \cdot_p a).$$

Using the commutative and associative laws for multiplication in Z_p and Equation 2.10, we get

$$1 \cdot_p 2 \cdot_p \cdots \cdot_p (p-1) = 1 \cdot_p 2 \cdot_p \cdots \cdot_p (p-1) \cdot_p (a^{p-1} \bmod p).$$

Now we multiply both sides of the equation by the multiplicative inverses in Z_p of 2, 3, …, $p-1$ and the left hand side of our equation becomes 1 and the right hand side becomes $a^{p-1} \bmod p$. But this is exactly the conclusion of our theorem. ■

Corollary 2.22 *(Fermat's Little Theorem, version 2) For every positive integer a, and prime p, if a is not a multiple of p,*

$$a^{p-1} \bmod p = 1.$$

Proof: This is a direct application of Lemma 2.3, because if we replace a by $a \bmod p$, then Theorem 2.21 applies.

The RSA Cryptosystem

Fermat's Little Theorem is at the heart of the RSA cryptosystem, a system that allows Bob to tell the world a way that they can encode a message to send to him so that he and only he can read it. In other words, even though he tells everyone how to encode the message, nobody except Bob has a significant chance of figuring out what the message is from looking at the encoded message. What Bob is giving out is called a "one-way function." This is a function f that has an inverse f^{-1}, but even though $y = f(x)$ is reasonably easy to compute, nobody but Bob (who has some extra information that he keeps secret) can compute $f^{-1}(y)$. Thus when Alice wants to send a message x to Bob, she computes $f(x)$ and sends it to Bob, who uses his secret information to compute $f^{-1}(f(x)) = x$.

In the RSA cryptosystem Bob chooses two prime numbers p and q (which in practice each have at least a hundred digits) and computes the number $n = pq$. He also chooses a number $e \neq 1$ which need not have a large number of digits but is relatively prime to $(p-1)(q-1)$, so that it has an inverse d in $Z_{(p-1)(q-1)}$, and he computes $d = e^{-1} \bmod (p-1)(q-1)$. Bob publishes e and n. The number e is called his *public key*. The number d is called his *private key*.

To summarize what we just said, here is a pseudocode outline of what Bob does:

<u>`Bob's RSA key choice algorithm`</u>
(1) `Choose 2 large prime numbers` p `and` q
(2) `n = pq`
(3) `Choose` $e \neq 1$ `so that` e `is relatively prime to` $(p-1)(q-1)$
(4) `Compute` $d = e^{-1} \bmod (p-1)(q-1)$.
(5) `Publish` e `and` n.
(6) `Keep` d `secret.`

People who want to send a message x to Bob compute $y = x^e \bmod n$ and send that to him instead. (We assume x has fewer digits than n so that it is in Z_n. If not, the sender has to break the message into blocks of size less than the number of digits of n and send each block individually.)

To decode the message, Bob will compute $z = y^d \bmod n$.

We summarize this process in pseudocode below:

<u>`Alice-send-message-to-Bob(`x`)`</u>
`Alice does:`
(1) `Read the public directory for Bob's keys` e `and` n.
(2) `Compute` $y = x^e \bmod n$

```
(3)       Send y to Bob
Bob does:
(4)   Receive y from Alice
(5)   Compute z = y^d mod n, using secret key d
(6)   Read z
```

Each step in these algorithms can be computed using methods from this chapter. In Section 2.4, we will deal with computational issues in more detail.

In order to show that the RSA cryptosystem works, that is, that it allows us to encode and then correctly decode messages, we must show that $z = x$. In other words, we must show that, when Bob decodes, he gets back the original message. In order to show that the RSA cryptosystem is secure, we must argue that an eavesdropper, who knows n, e, and y, but does not know p, q or d, can not easily compute x.

Exercise 2.3-5 To show that the RSA cryptosystem works, we will first show a simpler fact. Why is

$$y^d \bmod p = x \bmod p?$$

Does this tell us what x is?

Plugging in the value of y, we have

$$y^d \bmod p = x^{ed} \bmod p. \tag{2.14}$$

But, in Line 4 we chose e and d so that $e \cdot_m d = 1$, where $m = (p-1)(q-1)$. In other words,

$$ed \bmod (p-1)(q-1) = 1.$$

Therefore, for some integer k,

$$ed = k(p-1)(q-1) + 1.$$

Plugging this into Equation (2.14), we obtain

$$\begin{aligned} x^{ed} \bmod p &= x^{k(p-1)(q-1)+1} \bmod p \\ &= x^{(k(q-1))(p-1)} x \bmod p. \end{aligned} \tag{2.15}$$

But for any number a which is not a multiple of p, $a^{p-1} \bmod p = 1$ by Fermat's Little Theorem (Theorem 2.22). We could simplify equation 2.15 by applying Fermat's Little Theorem to $x^{k(q-1)}$, as you will see below. However we can only do this when $x^{k(q-1)}$ is not a multiple of p. This gives us two cases, the case in which $x^{k(q-1)}$ is not a multiple of p (we'll call this case 1) and the case in which $x^{k(q-1)}$ is a multiple of p (we'll call this case 2). In case 1, we apply Equation 2.12 and Fermat's Little Theorem with a equal to $x^{k(q-1)}$, and we have that

$$\begin{aligned} x^{(k(q-1))(p-1)} \bmod p &= \left(x^{k(q-1)}\right)^{(p-1)} \bmod p \\ &= 1. \end{aligned} \tag{2.16}$$

Combining equations 2.14, 2.15 and 2.17, we have that

$$y^d \bmod p = x^{k(q-1)(p-1)} x \bmod p = 1 \cdot x \bmod p = x \bmod p,$$

and hence $y^d \bmod p = x \bmod p$.

We still have to deal with case 2, the case in which $x^{k(q-1)}$ is a multiple of p. In this case x is a multiple of p as well since x is an integer and p is prime. Thus $x \bmod p = 0$. Combining Equations 2.14 and 2.15 with Lemma 2.3, we get

$$y^d \bmod p = (x^{k(q-1)(p-1)} \bmod p)(x \bmod p) = 0 = x \bmod p.$$

Hence in this case as well, we have $y^d \bmod p = x \bmod p$.

While this will turn out to be useful information, it does not tell us what x is, however, because x may or may not equal $x \bmod p$.

The same reasoning shows us that $y^d \bmod q = x \bmod q$. What remains is to show what these two facts tell us about $y^d \bmod pq = y \bmod n$, which is what Bob computes.

Notice that by Lemma 2.3 we have proved that

$$(y^d - x) \bmod p = 0 \tag{2.17}$$

and

$$(y^d - x) \bmod q = 0. \tag{2.18}$$

Exercise 2.3-6 Write down an equation using only integers and addition, subtraction and multiplication in the integers, but perhaps more letters, that is equivalent to Equation 2.17, which says that $(y^d - x) \bmod p = 0$. (Do not use mods.)

Exercise 2.3-7 Write down an equation using only integers and addition, subtraction and multiplication in the integers, but perhaps more letters, that is equivalent to Equation 2.18, which says that $(y^d - x) \bmod q = 0$. (Do not use mods.)

Exercise 2.3-8 If a number is a multiple of a prime p and a different prime q, then what else is it a multiple of? What does this tell us about y^d and x?

The statement that $y^d - x \bmod p = 0$ is equivalent to the statement that $y^d - x = ip$ for some integer i. The statement that $y^d - x \bmod q = 0$ is equivalent to the statement that $y^d - x = jq$ for some integer j. If something is a multiple of the prime p and the prime q, then it is a multiple of pq. Thus $(y^d - x) \bmod pq = 0$. Lemma 2.3 tells us that $(y^d - x) \bmod pq = (y^d \bmod pq - x) \bmod pq = 0$. But x and $y^d \bmod pq$ are both integers between 0 and $pq - 1$, so their difference is between $-(pq-1)$ and $pq - 1$. The only integer between these two values that is 0 mod pq is zero itself. Thus $(y^d \bmod pq) - x = 0$. In other words,

$$\begin{aligned} x &= y^d \bmod pq \\ &= y^d \bmod n \ , \end{aligned}$$

which means that Bob will in fact get the correct answer.

Theorem 2.23 *(Rivest, Shamir, and Adleman) The RSA procedure for encoding and decoding messages works correctly.*

Proof: Proved above.■

One might ask, given that Bob published e and n, and messages are encrypted by computing $x^e \bmod n$, why can't any adversary who learns $x^e \bmod n$ just compute eth roots mod n and break the code? At present, nobody knows a quick scheme for computing eth roots mod n, for an arbitrary n. Someone who does not know p and q cannot duplicate Bob's work and discover x. Thus, as far as we know, modular exponentiation is an example of a one-way function.

The Chinese Remainder Theorem

The method we used to do the last step of the proof of Theorem 2.23 also proves a theorem known as the "Chinese Remainder Theorem."

Exercise 2.3-9 For each number in $x \in Z_{15}$, write down $x \bmod 3$ and $x \bmod 5$. Is x uniquely determined by these values? Can you explain why?

x	$x \bmod 3$	$x \bmod 5$
0	0	0
1	1	1
2	2	2
3	0	3
4	1	4
5	2	0
6	0	1
7	1	2
8	2	3
9	0	4
10	1	0
11	2	1
12	0	2
13	1	3
14	2	4

Table 2.2: The values of $x \bmod 3$ and $x \bmod 5$ for each x between zero and 14.

As we see from Table 2.2, each of the $3 \cdot 5 = 15$ pairs (i, j) of integers i, j with $0 \le i \le 2$ and $0 \le j \le 4$ occurs exactly once as x ranges through the fifteen integers from 0 to 14. Thus the function f given by $f(x) = (x \bmod 3, x \bmod 5)$ is a one-to-one function from a fifteen element set to a fifteen element set, so each x is uniquely determined by its pair of remainders.

The Chinese Remainder Theorem tells us that this observation always holds.

Theorem 2.24 *(Chinese Remainder Theorem) If m and n are relatively prime integers and $a \in Z_m$ and $b \in Z_n$, then the equations*

$$x \bmod m = a \tag{2.19}$$

$$x \bmod n = b \tag{2.20}$$

have one and only one solution for an integer x between 0 and $mn - 1$.

Proof: If we show that as x ranges over the integers from 0 to $mn - 1$, then the ordered pairs $(x \bmod m, x \bmod n)$ are all different, then we will have shown that the function given by $f(x) = (x \bmod m, x \bmod n)$ is a one to one function from an mn element set to an mn element set, so it is onto as well.[7] In other words, we will have shown that each pair of equations 2.19 and 2.20 has one and only one solution.

In order to show that f is one-to-one, we must show that if x and y are different numbers between 0 and $mn-1$, then $f(x)$ and $f(y)$ are different. To do so, assume instead that we have an x and y with $f(x) = f(y)$. Then $x \bmod m = y \bmod m$ and $x \bmod n = y \bmod n$, so that $(x-y) \bmod m = 0$ and $(x-y) \bmod n = 0$. That is, $x-y$ is a multiple of both m and n. Then as we show in Problem 11 in the problems at the end of this section, $x-y$ is a multiple of mn; that is, $x-y = dmn$ for some integer d. Since we assumed x and y were different, this means x and y cannot both be between 0 and $mn-1$ because their difference is mn or more. This contradicts our hypothesis that x and y were different numbers between 0 and $mn-1$, so our assumption must be incorrect; that is f must be one-to-one. This completes the proof of the theorem. ■

Important Concepts, Formulas, and Theorems

1. *Exponentiation in Z_n.* For $a \in Z_n$, and a positive integer j:
$$a^j \bmod n = \underbrace{a \cdot_n a \cdot_n \cdots \cdot_n a}_{j \text{ factors}}.$$

2. *Rules of exponents.* For any $a \in Z_n$, and any nonnegative integers i and j,
$$(a^i \bmod n) \cdot_n (a^j \bmod n) = a^{i+j} \bmod n$$
and
$$\left(a^i \bmod n\right)^j \bmod n = a^{ij} \bmod n.$$

3. *Multiplication by a fixed nonzero a in Z_p is a permutation.* Let p be a prime number. For any fixed nonzero number a in Z_p, the numbers $(1\cdot a) \bmod p$, $(2\cdot a) \bmod p$, ..., $((p-1)\cdot a) \bmod p$, are a permutation of the set $\{1, 2, \cdots, p-1\}$.

4. *Fermat's Little Theorem.* Let p be a prime number. Then $a^{p-1} \bmod p = 1$ for each nonzero a in Z_p.

5. *Fermat's Little Theorem, version 2.* For every positive integer a and prime p, if a is not a multiple of p, then
$$a^{p-1} \bmod p = 1.$$

6. *RSA cryptosystem.* (The first implementation of a public-key cryptosystem) In the RSA cryptosystem Bob chooses two prime numbers p and q (which in practice each have at least a hundred digits) and computes the number $n = pq$. He also chooses a number $e \neq 1$ which need not have a large number of digits but is relatively prime to $(p-1)(q-1)$, so that it has an inverse d, and he computes $d = e^{-1} \bmod (p-1)(q-1)$. Bob publishes e and n. To send a message x to Bob, Alice sends $y = x^e \bmod n$. Bob decodes by computing $y^d \bmod n$.

[7]If the function weren't onto, then because the number of pairs is the same as the number of possible x-values, two x values would have to map to the same pair, so the function wouldn't be one-to-one after all.

7. *Chinese Remainder Theorem.* If m and n are relatively prime integers and $a \in Z_m$ and $b \in Z_n$, then the equations

$$\begin{aligned} x \bmod m &= a \\ x \bmod n &= b \end{aligned}$$

have one and only one solution for an integer x between 0 and $mn - 1$.

Problems

1. Compute the powers of 4 in Z_7. Compute the powers of 4 in Z_{10}. What is the most striking similarity? What is the most striking difference?

2. Compute the numbers $1 \cdot_{11} 5$, $2 \cdot_{11} 5$, $3 \cdot_{11} 5$, $\ldots$, $10 \cdot_{11} 5$. Do you get a permutation of the set $\{1,2,3,4,5,6,7,8,9,10\}$? Would you get a permutation of the set $\{1,2,3,4,5,6,7,8,9,10\}$ if you used another nonzero member of of Z_{11} in place of 5?

3. Compute the fourth power mod 5 of each element of Z_5. What do you observe? What general principle explains this observation?

4. The numbers 29 and 43 are primes. What is $(29-1)(43-1)$? What is $199 \cdot 1111$ in Z_{1176}? What is $(23^{1111})^{199}$ in Z_{29}? In Z_{43}? In Z_{1247}?

5. The numbers 29 and 43 are primes. What is $(29-1)(43-1)$? What is $199 \cdot 1111$ in Z_{1176}? What is $(105^{1111})^{199}$ in Z_{29}? In Z_{43}? In Z_{1247}? How does this answer the second question in Exercise 2.3-5?

6. How many solutions with x between 0 and 34 are there to the system of equations

$$\begin{aligned} x \bmod 5 &= 4 \\ x \bmod 7 &= 5? \end{aligned}$$

What are these solutions?

7. Compute each of the following. Show or explain your work, and do not use a calculator or computer.

   (a) 15^{96} in Z_{97}

   (b) 67^{72} in Z_{73}

   (c) 67^{73} in Z_{73}

8. Show that in Z_p, with p prime, if $a^i \bmod p = 1$, then $a^n \bmod p = a^{n \bmod i} \bmod p$.

9. Show that there are $p^2 - p$ elements with multiplicative inverses in Z_{p^2} when p is prime. If x has a multiplicative inverse in Z_p^2, what is $x^{p^2-p} \bmod p^2$? Is the same statement true for an element without an inverse? (Working out an example might help here.) Can you find something (interesting) that is true about x^{p^2-p} when x does not have an inverse?

10. How many elements have multiplicative inverses in Z_{pq} when p and q are primes?

11. In the paragraph preceding the proof of Theorem 2.23 we said that if a number is a multiple of the prime p and the prime q, then it is a multiple of pq. We will see how that is proved here.
    (a) What equation in the integers does Euclid's extended GCD algorithm solve for us when m and n are relatively prime?
    (b) Suppose that m and n are relatively prime and that k is a multiple of each one of them; that is, $k = bm$ and $k = cn$ for integers b and c. If you multiply both sides of the equation in part (a) by k, you get an equation expressing k as a sum of two products. By making appropriate substitutions in these terms, you can show that k is a multiple of mn. Do so. Does this justify the assertion we made in the paragraph preceding the proof of Theorem 2.23?
12. The relation of "congruence modulo n" is the relation $\equiv$ defined by $x \equiv y \bmod n$ if and only if $x \bmod n = y \bmod n$.
    (a) Show that congruence modulo n is an equivalence relation by showing that it defines a partition of the integers into equivalence classes.
    (b) Show that congruence modulo n is an equivalence relation by showing that it is reflexive, symmetric, and transitive.
    (c) Express the Chinese Remainder theorem in the notation of congruence modulo n.
13. Write and implement code to do RSA encryption and decryption. Use it to send a message to someone else in the class. (You may use smaller numbers than are usually used in implementing the RSA algorithm for the sake of efficiency. In other words, you may choose your numbers so that your computer can multiply them without overflow.)
14. For some non-zero $a \in Z_p$, where p is prime, consider the set
$$S = \{a^0 \bmod p,\ a^1 \bmod p,\ a^2 \bmod p,\ \ldots,\ a^{p-2} \bmod p,\ a^{p-1} \bmod p\},$$
and let $s = |S|$. Show that s is always a factor of $p - 1$.
15. Show that if $x^{n-1} \bmod n = 1$ for all integers x that are not multiples of n, then n is prime. (The slightly weaker statement that $x^{n-1} \bmod n = 1$ for all x relatively prime to n, does not imply that n is prime. There is a famous family of numbers called Carmichael numbers that are counterexamples.[8])

[8] See, for example, Cormen, Leiserson, Rivest, and Stein, cited earlier.

2.4 Details of the RSA Cryptosystem

In this section, we deal with some issues related to implementing the RSA cryptosystem: exponentiating large numbers, finding primes, and factoring.

Practical Aspects of Exponentiation mod n

Suppose you are going to raise a 100 digit number a to the 10^{120}th power modulo a 200 digit integer n. Note that the exponent is a 121 digit number.

Exercise 2.4-1 Propose an algorithm to compute $a^{10^{120}} \bmod n$, where a is a 100 digit number and n is a 200 digit number.

Exercise 2.4-2 What can we say about how long this algorithm would take on a computer that can do one infinite precision arithmetic operation in constant time?

Exercise 2.4-3 What can we say about how long this would take on a computer that can multiply integers in time proportional to the product of the number of digits in the two numbers, i.e. multiplying an x-digit number by a y-digit number takes roughly xy time?

Notice that if we form the sequence a, a^2, a^3, a^4, a^5, a^6, a^7, a^8, a^9, a^{10}, a^{11} we are modeling the process of forming a^{11} by successively multiplying by a. If, on the other hand, we form the sequence a, a^2, a^4, a^8, a^{16}, a^{32}, a^{64}, a^{128}, a^{256}, a^{512}, a^{1024}, we are modeling the process of successive squaring, and in the same number of multiplications we are able to get a raised to a four digit number. Each time we square we double the exponent, so every ten steps or so we will add three to the number of digits of the exponent. Thus in a bit under 400 multiplications, we will get $a^{10^{120}}$. This suggests that our algorithm should be to square a some number of times until the result is almost $a^{10^{120}}$, and then multiply by some smaller powers of a until we get exactly what we want. More precisely, we square a and continue squaring the result until we get the largest $a^{2^{k_1}}$ such that 2^{k_1} is less than 10^{120}, then multiply $a^{2^{k_1}}$ by the largest $a^{2^{k_2}}$ such that $2^{k_1} + 2^{k_2}$ is less than 10^{120} and so on until we have

$$10^{120} = 2^{k_1} + 2^{k_2} + \cdots + 2^{k_r}$$

for some integer r. (Can you connect this with the binary representation of 10^{120}?) Then we get

$$a^{10^{120}} = a^{2^{k_1}} a^{2^{k_2}} \cdots a^{2^{k_r}}.$$

Notice that all these powers of a have been computed in the process of discovering k_1. Thus it makes sense to save them as you compute them.

To be more concrete, let's see how to compute a^{43}. We may write $43 = 32 + 8 + 2 + 1$, and thus

$$a^{43} = a^{2^5} a^{2^3} a^{2^1} a^{2^0} \ . \tag{2.21}$$

So, we first compute $a^{2^0}, a^{2^1}, a^{2^2}, a^{2^3}, a^{2^4}, a^{2^5}$, using 5 multiplications. Then we can compute a^{43}, via equation 2.21, using 3 additional multiplications. This saves a large number of multiplications.

On a machine that could do infinite precision arithmetic in constant time, we would need about $\log_2(10^{120})$ steps to compute all the powers a^{2^i}, and perhaps equally many steps to do the multiplications of the appropriate powers. At the end we could take the result mod n. Thus the length of time it would take to do these computations would be more or less $2\log_2(10^{120}) = 240\log_2 10$ times the time needed to do one operation. (Since $\log_2 10$ is about 3.33, it will take at most 800 times the amount of time for one operation to compute $a^{10^{120}}$.)

You may not be used to thinking about how large the numbers get when you are doing computation. Computers hold fairly large numbers (4-byte integers in the range roughly -2^{31} to 2^{31} are typical), and this suffices for most purposes. Because of the way computer hardware works, as long as numbers fit into one 4-byte integer, the time to do simple arithmetic operations doesn't depend on the value of the numbers involved. (A standard way to say this is to say that the time to do a simple arithmetic operation is constant.) However, when we talk about numbers that are much larger than 2^{31}, we have to take special care to implement our arithmetic operations correctly, and also we have to be aware that operations are slower.

Since $2^{10} = 1024$, we have that 2^{31} is twice as big as $2^{30} = (2^{10})^3 = (1024)^3$ and so is somewhat more than two billion, or $2 \cdot 10^9$. In particular, it is less than 10^{10}. Since 10^{120} is a one followed by 120 zeros, raising a positive integer other than one to the 10^{120}th power takes us completely out of the realm of the numbers that we are used to making exact computations with. For example, $10^{(10^{120})}$ has 119 more zeros following the 1 in the exponent than does 10^{10}.

It is accurate to assume that when multiplying large numbers, the time it takes is roughly proportional to the product of the number of digits in each. If we computed our 100 digit number to the 10^{120}th power, we would be computing a number with more than 10^{120} digits. We clearly do **not** want to be doing computation on such numbers, as our computer cannot even store such a number!

Fortunately, since the number we are computing will ultimately be taken modulo some 200 digit number, we can make all our computations modulo that number. (See Lemma 2.3.) By doing so, we ensure that the two numbers we are multiplying together have at most 200 digits, and so the time needed for the problem proposed in Exercise 2.4-1 would be a proportionality constant times 40,000 times $\log_2(10^{120})$ times the time needed for a basic operation plus the time needed to figure out which powers of a are multiplied together, which would be quite small in comparison.

This algorithm, on 200 digit numbers, could be on the order of a million times slower than on simple integers.[9] This is a noticeable effect and if you use or write an encryption program, you can see this effect when you run it. However, we can still typically do this calculation in less than a second, a small price to pay for secure communication.

How long does it take to use the RSA Algorithm?

Encoding and decoding messages according to the RSA algorithm requires many calculations. How long will all this arithmetic take? Let's assume for now that Bob has already chosen p, q, e, and d, and so he knows n as well. When Alice wants to send Bob the message x, she

[9] If we assume that we can multiply four digit integers exactly but not five digit numbers exactly, then efficiently multiplying two 200 digit numbers is like multiplying 50 integers times 50 integers, or 2500 products, and $\log_2(10^{120}) \approx \log_2((2^10)^{40} = \log_2(2^{400}) = 400$, so we would have something like million steps, each equivalent to multiplying two integers, in executing our algorithm.

sends $x^e \bmod n$. By our analyses in Exercise 2.4-2 and Exercise 2.4-3 we see that this amount of time is more or less proportional to $\log_2 e$, which is itself proportional to the number of digits of e, though the first constant of proportionality depends on the method our computer uses to multiply numbers. Since e has no more than 200 digits, this should not be too time consuming for Alice if she has a reasonable computer. (On the other hand, if she wants to send a message consisting of many segments of 200 digits each, she might want to use the RSA system to send a key for another simpler (secret key) system, and then use that simpler system for the message.)

It takes Bob a similar amount of time to decode, as he has to take the message to the dth power, mod n.

We commented already that nobody knows a fast way to find x from $x^e \bmod n$. In fact, nobody knows that there isn't a fast way either, which means that it is possible that the RSA cryptosystem could be broken some time in the future. We also don't know whether extracting eth roots mod n is in the class of #P-complete problems, an important family of problems with the property that a reasonably fast solution of any one of them will lead to a reasonably fast solution of any of them. We do know that extracting eth roots is no harder than these problems, but it may be easier.

However, here someone is not restricted to extracting roots to discover x. Someone who knows n and knows that Bob is using the RSA system, could presumably factor n, discover p and q, use the extended GCD algorithm to compute d and then decode all of Bob's messages. However, nobody knows how to factor integers quickly either. Again, we don't know if factoring is #P-complete, but we do know that it is no harder than the #P-complete problems. Thus here is a second possible way around the RSA system. However, enough people have worked on the factoring problem that most compputer scientists are confident that it is in fact difficult, in which case the RSA system is safe, as long as we use keys that are long enough.

How hard is factoring?

Exercise 2.4-4 Factor 225,413. (The idea is to try to do this without resorting to computers, but if you give up by hand and calculator, using a computer is fine.)

With current technology, keys with roughly 100 digits are not that hard to crack. In other words, people can factor numbers that are roughly 100 digits long, using methods that are a little more sophisticated than the obvious approach of trying all possible divisors. However, when the numbers get long, say over 120 digits, they become very hard to factor. The record, as of the year 2000, for factoring is a roughly 155-digit number. To factor this number, thousands of computers around the world were used, and it took several months. So given the current technology, RSA with a 200 digit key seems to be very secure.

Finding large primes

There is one more issue to consider in implementing the RSA system for Bob. We said that Bob chooses two primes of about a hundred digits each. But how does he choose them? It follows from some celebrated work on the density of prime numbers that if we were to choose a number m at random, and check about $\log_e(m)$ numbers around m for primality, we would expect that one of these numbers was prime. Thus if we have a reasonably quick way to check whether a number is prime, we shouldn't have to guess too many numbers, even with a hundred or so digits, before we find one we can show is prime.

However, we have just mentioned that nobody knows a quick way to find any or all factors of a number. The standard way of proving a number is prime is by showing that it and 1 are its only factors. For the same reasons that factoring is hard, the simple approach to primality testing, test all possible divisors, is much too slow. If we did not have a faster way to check whether a number is prime, the RSA system would be useless.

In August of 2002, Agrawal, Kayal and Saxena announced an algorithm for testing whether an integer n is prime which they can show takes no more than the twelveth power of the number of digits of n to determine whether n is prime, and in practice seems to take significantly less time. While the algorithm requires more than the background we are able to provide in this book, its description and the proof that it works in the specified time uses only results that one might find in an undergraduate abstract algebra course and an undergraduate number theory course! The central theme of the algorithm is the use of a variation of Fermat's Little Theorem.

In 1976 Miller[10] was able to use Fermat's Little Theorem to show that if a conjecture called the "Extended Reiman Hypothesis" was true, then an algorithm he developed would determine whether a number n was prime in a time bounded above by a polynomial in the number of digits of n. In 1980 Rabin[11] modified Miller's method to get one that would determine in polynomial time whether a number was prime without the extra hypothesis, but with a probability of error that could be made as small a positive number as one might desire, but not zero. We describe the general idea behind all of these advances in the context of what people now call the Miller-Rabin primality test. As of the writing of this book, variations on this kind of algorithm are used to provide primes for cryptography.

We know, by Fermat's Little Theorem, that in Z_p with p prime, $x^{p-1} \bmod p = 1$ for every x between 1 and $p-1$. What about x^{m-1}, in Z_m, when m is not prime?

Exercise 2.4-5 Suppose x is a member of Z_m that has no multiplicative inverse. Is it possible that $x^{n-1} \bmod n = 1$?

We answer the question of the exercise in our next lemma.

Lemma 2.25 *Let m be a non-prime, and let x be a number in Z_m which has no multiplicative inverse. Then $x^{m-1} \bmod m \neq 1$.*

Proof: Assume, for the purpose of contradiction, that

$$x^{m-1} \bmod m = 1.$$

Then

$$x \cdot x^{m-2} \bmod m = 1.$$

But then $x^{m-2} \bmod m$ is the inverse of x in Z_m, which contradicts the fact that x has no multiplicative inverse. Thus it must be the case that $x^{m-1} \bmod m \neq 1$. ■

[10]G.L. Miller. "Riemann's Hypothesis and tests for primality," J. Computer and Systems Science **13**, 1976, pp 300-317.

[11]M. O. Rabin. "Probabilistic algorithm for testing primality." Journal of Number Theory, **12**, 1980. pp 128-138.

This distinction between primes and non-primes gives the idea for an algorithm. Suppose we have some number m, and are not sure whether it is prime or not. We can run the following algorithm:

```
PrimeTest(m)
choose a random number x, 2 ≤ x ≤ m − 1.
compute y = x^(m−1) mod m
if (y = 1)
      output `` m might be prime''
else
      output ``m is definitely not prime''
```

Note the asymmetry here. If $y \neq 1$, then m is definitely not prime, and we are done. On the other hand, if $y = 1$, then the m might be prime, and we probably want to do some other calculations. In fact, we can repeat the algorithm Primetest(m) for t times, with a different random number x each time. If on any of the t runs, the algorithm outputs "m is definitely not prime", then the number m is definitely not prime, as we have an x for which $x^{m-1} \neq 1$. On the other hand, if on all t runs, the algorithm Primetest(m) outputs "m might be prime", then, with reasonable certainty, we can say that the number m is prime. This is actually an example of a *randomized algorithm*; we will be studying these in greater detail later in the course. For now, let's informally see how likely it is that we make a mistake.

We can see that the chance of making a mistake depends on, for a particular non-prime m, exactly how many numbers a have the property that $a^{m-1} = 1$. If the answer is that very few do, then our algorithm is very likely to give the correct answer. On the other hand, if the answer is most of them, then we are more likely to give an incorrect answer.

In Exercise 12 at the end of the section, you will show that the number of elements in Z_m without inverses is at least $\sqrt{m}$. In fact, even many numbers that do have inverses will also fail the test $x^{m-1} = 1$. For example, in Z_{12} only 1 passes the test while in Z_{15} only 1 and 14 pass the test. (Z_{12} really is not typical; can you explain why? See Problem 13 at the end of this section for a hint.)

In fact, the Miller-Rabin algorithm modifies the test slightly (in a way that we won't describe here[12]) so that for any non-prime m, at least half of the possible values we could choose for x will fail the modified test and hence will show that m is composite. As we will see when we learn about probability, this implies that if we repeat the test t times, and assert that an x which passes these t tests is prime, the probability of being wrong is actually 2^{-t}. So, if we repeat the test 10 times, we have only about a 1 in a thousand chance of making a mistake, and if we repeat it 100 times, we have only about a 1 in 2^{100} (a little less than one in a nonillion) chance of making a mistake!

Numbers we have chosen by this algorithm are sometimes called *pseudoprimes*. They are called this because they are very likely to be prime. In practice, pseudoprimes are used instead of primes in implementations of the RSA cryptosystem. The worst that can happen when a pseudoprime is not prime is that a message may be garbled; in this case we know that our pseudoprime is not really prime, and choose new pseudoprimes and ask our sender to send the

[12] See, for example, Cormen, Leiserson, Rivest and Stein, Introduction to Algorithms, McGraw Hill/MIT Press, 2002

message again. (Note that we do not change p and q with each use of the system; unless we were to receive a garbled message, we would have no reason to change them.)

A number theory theorem called the Prime Number Theorem tells us that if we check about $\log_e n$ numbers near n we can expect one of them to be prime. A d digit number is at least 10^{d-1} and less than 10^d, so its natural logarithm is between $(d-1)\log_e 10$ and $d\log_e 10$. If we want to find a d digit prime, we can take any d digit number and test about $d\log_e 10$ numbers near it for primality, and it is reasonable for us to expect that one of them will turn out to be prime. The number $\log_e 10$ is 2.3 to two decimal places. Thus it does not take a really large amount of time to find two prime numbers with a hundred (or so) digits each.

Important Concepts, Formulas, and Theorems

1. *Exponentiation.* To perform exponentiation mod n efficiently, we use repeated squaring, and take mods after each arithmetic operation.
2. *Security of RSA.* The security of RSA rests on the fact that no one has developed an efficient algorithm for factoring, or for finding x, given x^e mod n.
3. *Fermat's Little Theorem does not hold for composites.* Let m b e a non-prime, and let x be a number in Z_n which has no multiplicative inverse. Then $x^{m-1} \bmod m \neq 1$.
4. *Testing numbers for primality.* The randomized Miller-Rabin algorithm will tell you almost surely if a given number is prime.
5. *Finding prime numbers.* By applying the randomized Miller-Rabin to $d\ln 10$ (which is about $2.3d$) numbers with d digits, you can expect to find at least one that is prime.

Problems

1. What is 3^{1024} in Z_7? (This is a straightforward problem to do by hand.)
2. Suppose we have computed a^2, a^4, a^8, a^{16} and a^{32}. What is the most efficient way for us to compute a^{53}?
3. A gigabyte is one billion bytes; a terabyte is one trillion bytes. A byte is eight bits, each a zero or a 1. Since $2^{10} = 1024$, which is about 1000, we can store about three digits (any number between 0 and 999) in ten bits. About how many decimal digits could we store in a five gigabytes of memory? About how many decimal digits could we store in five terabytes of memory? How does this compare to the number 10^{120}? To do this problem it is reasonable to continue to assume that 1024 is about 1000.
4. Find all numbers a different from 1 and -1 (which is the same as 8) such that $a^8 \bmod 9 = 1$.
5. Use a spreadsheet, programmable calculator or computer to find all numbers a different from 1 and $-1 \bmod 33 = 32$ with $a^{32} \bmod 33 = 1$. (This problem is relatively straightforward to do with a spreadsheet that can compute mods and will let you "fill in" rows and columns with formulas. However you do have to know how to use the spreadsheet in this way to make it strightforward!)

6. How many digits does the 10^{120}th power of 10^{100} have?

7. If a is a 100 digit number, is the number of digits of $a^{10^{120}}$ closer to 10^{120} or 10^{240}? Is it a lot closer? Does the answer depend on what a actually is rather than the number of digits it has?

8. Explain what our outline of the solution to Exercise 2.4-1 has to do with the binary representation of 10^{120}.

9. Give careful pseudocode to compute $a^x \bmod n$. Make your algorithm as efficient as possible. You may use right shift n in your algorithm.

10. Suppose we want to compute $a^{e_1 e_2 \cdots e_m} \bmod n$. Discuss whether it makes sense to reduce the exponents mod n as we compute their product. In particular, what rule of exponents would allow us to do this, and do you think this rule of exponents makes sense?

11. Number theorists use $\varphi(n)$ to stand for the number of elements of Z_n that have inverses. Suppose we want to compute $a^{e_1 e_2 \cdots e_m} \bmod n$. Would it make sense for us to reduce our exponents mod $\varphi(n)$ as we compute their product? Why?

12. Show that if m is not prime, then at least $\sqrt{m}$ elements of Z_m do not have multiplicative inverses.

13. Show that in Z_{p+1}, where p is prime, only one element passes the primality test $x^{m-1} = 1 \pmod{m}$. (In this case, $m = p + 1$.)

14. Suppose for RSA, $p = 11$, $q = 19$, and $e = 7$. What is the value of d? Show how to encrypt the message 100, and then show how to decrypt the resulting message.

15. Suppose for applying RSA, $p = 11$, $q = 23$, and $e = 13$. What is the value of d? Show how to encrypt the message 100 and then how to decrypt the resulting message.

16. A digital signature is a way to securely sign a document. That is, it is a way to put your "signature" on a document so that anyone reading it knows that it is you who have signed it, but no one else can "forge" your signature. The document itself may be public; it is your signature that we are trying to protect. Digital signatures are, in a way, the opposite of encryption, as if Bob wants to sign a message, he first applies his signature to it (think of this as encryption) and then the rest of the world can easily read it (think of this as decryption). Explain, in detail, how to achieve digital signatures, using ideas similar to those used for RSA. In particular, anyone who has the document and has your signature of the document (and knows your public key) should be able to determine that you signed it.

Chapter 3

Reflections on Logic and Proof

In this chapter, we cover some basic principles of logic and describe some methods for constructing proofs. This chapter is not meant to be a complete enumeration of all possible proof techniques. The philosophy of this book is that most people learn more about proofs by reading, watching, and attempting proofs than by an extended study of the logical rules behind proofs. On the other hand, now that we have some examples of proofs, it will help you read and do proofs if we reflect on their structure and discuss what constitutes a proof. To do so so we first develop a language that will allow us to talk about proofs, and then we use this language to describe the logical structure of a proof.

3.1 Equivalence and Implication

Equivalence of statements

Exercise 3.1-1 A group of students are working on a project that involves writing a merge sort program. Joe and Mary have each written an algorithm for a function that takes two lists, `List1` and `List2`, of lengths p and q and merges them into a third list, `List3`. Part of Mary's algorithm is the following:

(1) `if` $((i+j \leq p+q)$ && $(i \leq p)$ && $((j \geq q) || (\texttt{List1}[i] \leq \texttt{List2}[j])))$
(2) $\qquad$ `List3`$[k]$ = `List1`$[i]$
(3) $\qquad$ $i = i+1$
(4) `else`
(5) $\qquad$ `List3`$[k]$ = `List2`$[j]$
(6) $\qquad$ $j = j+1$

(7) $k = k+1$
(8) `Return List3`

The corresponding part of Joe's algorithm is

(1) `if` $(((i+j \leq p+q)$ && $(i \leq p)$ && $(j \geq q))$
$\qquad ||$ $((i+j \leq p+q)$ && $(i \leq p)$ && $(\texttt{List1}[i] \leq \texttt{List2}[j])))$

```
(2)           List3[k] = List1[i]
(3)           i = i + 1
(4)   else
(5)           List3[k] = List2[j]
(6)           j = j + 1

(7)   k = k + 1
(8)   Return List3
```

Do Joe and Mary's algorithms do the same thing?

Notice that Joe and Mary's algorithms are exactly the same except for the if statement in line 1. (How convenient; they even used the same local variables!) In Mary's algorithm we put entry i of `List1` into position k of `List3` if

$$i + j \leq p + q \text{ and } i \leq p \text{ and } (j \geq q \text{ or } \texttt{List1}[i] \leq \texttt{List2}[j]),$$

while in Joe's algorithm we put entry i of `List1` into position k of `List3` if

$$(i+j \leq p+q \text{ and } i \leq p \text{ and } j \geq q) \text{ or } (i+j \leq p+q \text{ and } i \leq p \text{ and } \texttt{List1}[i] \leq \texttt{List2}[j]).$$

Joe and Mary's statements are both built up from the same constituent parts (namely comparison statements), so we can name these constituent parts and rewrite the statements. We use

- s to stand for $i + j \leq p + q$,
- t to stand for $i \leq p$,
- u to stand for $j \geq q$, and
- v to stand for $\texttt{List1}[i] \leq \texttt{List2}[j]$

The condition in Mary's if statement on Line 1 of her code becomes

$$s \text{ and } t \text{ and } (u \text{ or } v)$$

while Joe's if statement on Line 1 of his code becomes

$$(s \text{ and } t \text{ and } u) \text{ or } (s \text{ and } t \text{ and } v).$$

By recasting the statements in this symbolic form, we see that s and t always appear together as "s and t." We can thus simplify their expressions by substituting w for "s and t." Mary's condition now has the form

$$w \text{ and } (u \text{ or } v)$$

and Joe's has the form

(w and u) or (w and v).

Although we can argue, based on our knowledge of the structure of the English language, that Joe's statement and Mary's statement are saying the same thing, it will help us understand logic if we formalize the idea of "saying the same thing." If you look closely at Joe's and Mary's statements, you can see that we are saying that, the word "and" distributes over the word "or," just as set intersection distributes over set union, and multiplication distributes over addition. In order to analyze when statements mean the same thing, and explain more precisely what we mean when we say something like "and" distributes over "or," logicians have adopted a standard notation for writing symbolic versions of compound statements. We shall use the symbol $\wedge$ to stand for "and" and $\vee$ to stand for "or." In this notation, Mary's condition becomes

$$w \wedge (u \vee v)$$

and Joe's becomes

$$(w \wedge u) \vee (w \wedge v).$$

We now have a nice notation (which makes our compound statements look a lot like the two sides of the distributive law for intersection of sets over union), but we have not yet explained why two statements with this symbolic form mean the same thing. We must therefore give a precise definition of "meaning the same thing," and develop a tool for analyzing when two statements satisfy this definition. We are going to consider symbolic compound statements that may be built up from the following notation:

- symbols (s, t, etc.) standing for statements (these will be called *variables*),
- the symbol $\wedge$, standing for "and,"
- the symbol $\vee$, standing for "or,"
- the symbol $\oplus$ standing for "exclusive or," and
- the symbol $\neg$, standing for "not."

Truth tables

We will develop a theory for deciding when a compound statement is true based on the truth or falsity of its component statements. Using this theory, we will determine, for a particular setting of variables, say s, t and u, whether a particular compound statement, say $(s \oplus t) \wedge (\neg u \vee (s \wedge t)) \wedge \neg(s \oplus (t \vee u))$, is true or false. Our technique uses truth tables, which you have probably seen before. We will see how truth tables are the proper tool to determine whether two statements are equivalent.

As with arithmetic, the order of operations in a logical statement is important. In our sample compound statement $(s \oplus t) \wedge (\neg u \vee (s \wedge t)) \wedge \neg(s \oplus (t \vee u))$ we used parentheses to make it clear which operation to do first, with one exception, namely our use of the $\neg$ symbol. The symbol $\neg$ always has the highest priority, which means that when we wrote $\neg u \vee (s \wedge t)$, we meant $(\neg u) \vee (s \wedge t)$, rather than $\neg(u \vee (s \wedge t))$. The principle we use here is simple; the symbol $\neg$

applies to the smallest number of possible following symbols needed for it to make sense. This is the same principle we use with minus signs in algebraic expressions. With this one exception, we will always use parentheses to make the order in which we are to perform operations clear; you should do the same.

The operators $\wedge$, $\vee$, $\oplus$ and $\neg$ are called *logical connectives*. The truth table for a logical connective states, in terms of the possible truth or falsity of the component parts, when the compound statement made by connecting those parts is true and when it is false. The the truth tables for the connectives we have mentioned so far are in Figure 3.1

Figure 3.1: The truth tables for the basic logical connectives.

AND

s	t	$s \wedge t$
T	T	T
T	F	F
F	T	F
F	F	F

OR

s	t	$s \vee t$
T	T	T
T	F	T
F	T	T
F	F	F

XOR

s	t	$s \oplus t$
T	T	F
T	F	T
F	T	T
F	F	F

NOT

s	$s \oplus t$
T	F
F	T

These truth tables define the words "and," "or," "exclusive or" ("xor" for short), and "not" in the context of symbolic compound statements. For example, the truth table for $\vee$—or—tells us that when s and t are both true, then so is "s or t." It tells us that when s is true and t is false, or s is false and t is true, then "s or t" is true. Finally it tells us that when s and t are both false, then so is "s or t." Is this how we use the word "or" in English? The answer is sometimes! The word "or" is used ambiguously in English. When a teacher says "Each question on the test will be short answer or multiple choice," the teacher is presumably not intending that a question could be both. Thus the word "or" is being used here in the sense of "exclusive or"—the "$\oplus$" in the truth tables above. When someone says "Let's see, this afternoon I could take a walk or I could shop for some new gloves," she probably does not mean to preclude the possibility of doing both—perhaps even taking a walk downtown and then shopping for new gloves before walking back. Thus in English, we determine the way in which someone uses the word "or" from context. In mathematics and computer science we don't always have context and so we agree that we will say "exclusive or" or "xor" for short when that is what we mean, and otherwise we will mean the "or" whose truth table is given by $\vee$. In the case of "and" and "not" the truth tables are exactly what we would expect.

We have been thinking of s and t as variables that stand for statements. The purpose of a truth table is to define when a compound statement is true or false in terms of when its component statements are true and false. Since we focus on just the truth and falsity of our statements when we are giving truth tables, we can also think of s and t as variables that can take on the values "true" (T) and "false" (F). We refer to these values as the *truth values* of s and t. Then a truth table gives us the truth values of a compound statement in terms of the truth values of the component parts of the compound statement. The statements $s \wedge t$, $s \vee t$ and $s \oplus t$ each have two component parts, s and t. Because there are two values we can assign to s, and for each value we assign to s there are two values we can assign to t, by the product principle, there are $2 \cdot 2 = 4$ ways to assign truth values to s and t. Thus we have four rows in our truth table, one for each way of assigning truth values to s and t.

For a more complex compound statement, such as the one in Line 1 in Joe and Mary's programs, we still want to describe situations in which the statement is true and situations in

Table 3.1: The truth table for Joe's statement

w	u	v	$u \vee v$	$w \wedge (u \vee v)$
T	T	T	T	T
T	T	F	T	T
T	F	T	T	T
T	F	F	F	F
F	T	T	T	F
F	T	F	T	F
F	F	T	T	F
F	F	F	F	F

which the statement is false. We will do this by working out a truth table for the compound statement from the truth tables of its symbolic statements and its connectives. We use a variable to represent the truth value each symbolic statement. The truth table has one column for each of the original variables, and for each of the pieces we use to build up the compound statement. The truth table has one row for each possible way of assigning truth values to the original variables. Thus if we have two variables, we have, as above, four rows. If we have just one variable, then we have, as above, just two rows. If we have three variables then we will have $2^3 = 8$ rows, and so on.

In Table 3.1 we give the truth table for the symbolic statement that we derived from Line 1 of Joe's algorithm. The columns to the left of the double line contain the possible truth values of the variables; the columns to the right correspond to various sub-expressions whose truth values we need to compute. We give the truth table as many columns as we need in order to correctly compute the final result; as a general rule, each column should be easily computed from one or two previous columns.

In Table 3.2 we give the truth table for the statement that we derived from Line 1 of Mary's algorithm.

Table 3.2: The truth table for Mary's statement

w	u	v	$w \wedge u$	$w \wedge v$	$(w \wedge u) \vee (w \wedge v)$
T	T	T	T	T	T
T	T	F	T	F	T
T	F	T	F	T	T
T	F	F	F	F	F
F	T	T	F	F	F
F	T	F	F	F	F
F	F	T	F	F	F
F	F	F	F	F	F

You will notice that the pattern of T's and F's that we used to the left of the double line in both Joe's and Mary's truth tables are the same—namely, reverse alphabetical order.[1] Thus

[1]Alphabetical order is sometimes called *lexicographic order*. Lexicography is the study of the principles and

row i of Table 3.1 represents exactly the same assignment of truth values to u , v, and w as row i of Table 3.2. The final columns of the two truth tables are identical, which means that Joe's symbolic statement and Mary's symbolic statement are true in exactly the same cases. Therefore, the two statements must say the same thing, and Mary and Joe's program segments return exactly the same values. We say that two symbolic compound statements are *equivalent* if they are true in exactly the same cases. Alternatively, two statements are equivalent if their truth tables have the same final column (assuming both tables assign truth values to the original symbolic statements in the same pattern).

Tables 3.1 and 3.2 actually prove a *distributive law*:

Lemma 3.1 *The statements*

$$w \wedge (u \vee v)$$

and

$$(w \wedge u) \vee (w \wedge v)$$

are equivalent.

DeMorgan's Laws

Exercise 3.1-2 *DeMorgan's Laws* say that $\neg(p \vee q)$ is equivalent to $\neg p \wedge \neg q$, and that $\neg(p \wedge q)$ is equivalent to $\neg p \vee \neg q$,. Use truth tables to demonstrate that DeMorgan's laws are correct.

Exercise 3.1-3 Show that $p \oplus q$, the exclusive or of p and q, is equivalent to $(p \vee q) \wedge \neg(p \wedge q)$. Apply one of DeMorgan's laws to $\neg(\neg(p \vee q)) \wedge \neg(p \wedge q)$ to find another symbolic statement equivalent to the exclusive or.

To verify the first DeMorgan's Law, we create a pair of truth tables that we have condensed into one "double truth table" in Table 3.3. The second double vertical line separates the computation of the truth values of $\neg(p \vee q)$ and $\neg p \wedge \neg q$ We see that the fourth and the last columns are identical,

Table 3.3: Proving the first DeMorgan Law.

p	q	$p \vee q$	$\neg(p \vee q)$	$\neg p$	$\neg q$	$\neg p \wedge \neg q$
T	T	T	F	F	F	F
T	F	T	F	F	T	F
F	T	T	F	T	F	F
F	F	F	T	T	T	T

and therefore the first DeMorgan's Law is correct. We can verify the second of DeMorgan's Laws by a similar process.

To show that $p \oplus q$ is equivalent to $(p \vee q) \wedge \neg(p \wedge q)$, we use the "double truth table" in Table 3.4.

practices used in making dictionaries. Thus you will also see the order we used for the T's and F's called reverse lexicographic order, or reverse lex order for short.

Table 3.4: An equivalent statement to $p \oplus q$.

p	q	$p \oplus q$	$p \vee q$	$p \wedge q$	$\neg(p \wedge q)$	$(p \vee q) \wedge \neg(p \wedge q)$
T	T	F	T	T	F	F
T	F	T	T	F	T	T
F	T	T	T	F	T	T
F	F	F	F	F	T	F

By applying DeMorgan's law to $\neg(\neg(p \vee q)) \wedge \neg(p \wedge q)$, we see that $p \oplus q$ is also equivalent to $\neg(\neg(p \vee q) \vee (p \wedge q))$. It was easier to use DeMorgan's law to show this equivalence than to use another double truth table.

Implication

Another kind of compound statement occurs frequently in mathematics and computer science. Recall 2.21, Fermat's Little Theorem:

> If p is a prime, then $a^{p-1} \bmod p = 1$ for each non-zero $a \in Z_p$.

Fermat's Little Theorem combines two constituent statements,

> p is a prime

and

> $a^{p-1} \bmod p = 1$ for each non-zero $a \in Z_p$.

We can also restate Fermat's Little Theorem (a bit clumsily) as

> p is a prime only if $a^{p-1} \bmod p = 1$ for each non-zero $a \in Z_p$,

or

> p is a prime implies $a^{p-1} \bmod p = 1$ for each non-zero $a \in Z_p$,

or

> $a^{p-1} \bmod p = 1$ for each non-zero $a \in Z_p$ if p is prime.

Using s to stand for "p is a prime" and t to stand for "$a^{p-1} \bmod p = 1$ for every non-zero $a \in Z_p$," we symbolize any of the four statements of Fermat's Little Theorem as

$$s \Rightarrow t,$$

which most people read as "s implies t." When we translate from symbolic language to English, it is often clearer to say "If s then t."

We summarize this discussion in the following definition:

Definition 3.1 *The following four English phrases are intended to mean the same thing. In other words, they are defined by the same truth table:*

- *s implies t,*
- *if s then t,*
- *t if s, and*
- *s only if t.*

Observe that the use of "only if" may seem a little different than the normal usage in English. Also observe that there are still other ways of making an "if ... then" statement in English. In a number of our lemmas, theorems, and corollaries (for example, Corollary 2.6 and Lemma 2.5) we have had two sentences. In the first we say "Suppose ... ." In the second we say "Then ... ." The two sentences "Suppose s." and "Then t." are equivalent to the single sentence $s \Rightarrow t$. When we have a statement equivalent to $s \Rightarrow t$, we call the statement s the *hypothesis* of the implication and we call the statement t the *conclusion* of the implication.

If and only if

The word "if" and the phrase "only if" frequently appear together in mathematical statements. For example, in Theorem 2.9 we proved

> A number a has a multiplicative inverse in Z_n if and only if there are integers x and y such that $ax + ny = 1$.

Using s to stand for the statement "a number a has a multiplicative inverse in Z_n" and t to stand for the statement "there are integers x and y such that $ax+ny = 1$," we can write this statement symbolically as

> s if and only if t.

Referring to Definition 3.1, we parse this as

> s if t, and s only if t,

which again by the definition above is the same as

> $s \Rightarrow t$ and $t \Rightarrow s$.

We denote the statement "s if and only if t" by $s \Leftrightarrow t$. Statements of the form $s \Rightarrow t$ and $s \Leftrightarrow t$ are called *conditional statements*, and the connectives $\Rightarrow$ and $\Leftrightarrow$ are called *conditional connectives.*

Exercise 3.1-4 Use truth tables to explain the difference between $s \Rightarrow t$ and $s \Leftrightarrow t$.

In order to be able to analyze the truth and falsity of statements involving "implies" and "if and only if," we need to understand exactly how they are different. By constructing truth tables for these statements, we see that there is only one case in which they could have different truth values. In particular if s is true and t is true, then we would say that both $s \Rightarrow t$ and $s \Leftrightarrow t$ are true. If s is true and t is false, we would say that both $s \Rightarrow t$ and $s \Leftrightarrow t$ are false. In the case that both s and t are false we would say that $s \Leftrightarrow t$ is true. What about $s \Rightarrow t$? Let us try an example. Suppose that s is the statement "it is supposed to rain" and t is the statement "I carry an umbrella." Then if, on a given day, it is not supposed to rain and I do not carry an umbrella, we would say that the statement "if it is supposed to rain then I carry an umbrella" is true on that day. This suggests that we also want to say $s \Rightarrow t$ is true if s is false and t is false.[2] Thus the truth tables are identical in rows one, two, and four. For "implies" and "if and only if" to mean different things, the truth tables must therefore be different in row three. Row three is the case where s is false and t is true. Clearly in this case we would want s if and only if t to be false, so our only choice is to say that $s \Rightarrow t$ is true in this case. This gives us the truth tables in Figure 3.2.

Figure 3.2: The truth tables for "implies" and for "if and only if."

IMPLIES

s	t	$s \Rightarrow t$
T	T	T
T	F	F
F	T	T
F	F	T

IF AND ONLY IF

s	t	$s \Leftrightarrow t$
T	T	T
T	F	F
F	T	F
F	F	T

Here is another place where (as with the usage for "or") English usage is sometimes inconsistent. Suppose a parent says "I will take the family to McDougalls for dinner if you get an A on this test," and even though the student gets a C, the parent still takes the family to McDougalls for dinner. While this is something we didn't expect, was the parent's statement still true? Some people would say "yes"; others would say "no". Those who would say "no" mean, in effect, that in this context the parent's statement meant the same as "I will take the family to dinner at McDougalls if and only if you get an A on this test." In other words, to some people, in certain contexts, "If" and "If and only if" mean the same thing! Fortunately questions of child rearing aren't part of mathematics or computer science (at least not this kind of question!). In mathematics and computer science, we adopt the two truth tables just given as the meaning of the compound statement $s \Rightarrow t$ (or "if s then t" or "t if s") and the compound statement $s \Leftrightarrow t$ (or "s if and only if t.") In particular, the truth table marked IMPLIES is the truth table referred to in Definition 3.1. This truth table thus defines the mathematical meaning of s implies t, or any of the other three statements referred to in that definition.

Some people have difficulty using the truth table for $s \Rightarrow t$ because of this ambiguity in English. The following example can be helpful in resolving this ambiguity. Suppose that I hold

[2] Note that we are making this conclusion on the basis of one example. Why can we do so? We are not trying to prove something, but trying to figure out what the appropriate definition is for the $\Rightarrow$ connective. Since we have said that the truth or falsity of $s \Rightarrow t$ depends only on the truth or falsity of s and t, one example serves to lead us to an appropriate definition. If a different example led us to a different definition, then we would want to define two different kinds of implications, just as we have two different kinds of "ors," $\vee$ and $\oplus$. Fortunately, the only kinds of conditional statements we need for doing mathematics and computer science are "implies" and "if and only if."

an ordinary playing card (with its back to you) and say "If this card is a heart, then it is a queen." In which of the following four circumstances would you say I lied:

1. the card is a heart and a queen
2. the card is a heart and a king
3. the card is a diamond and a queen
4. the card is a diamond and a king?

You would certainly say I lied in the case the card is the king of hearts, and you would certainly say I didn't lie if the card is the queen of hearts. Hopefully in this example, the inconsistency of English language seems out of place to you and you would not say I am a liar in either of the other cases. Now we apply the principle called the *principle of the excluded middle*

Principle 3.1 *A statement is true exactly when it is not false.*

This principle tells us that that my statement is true in the three cases where you wouldn't say I lied. We used this principle implicitly before when we introduced the principle of proof by contradiction, Principle 2.1. We were explaining the proof of Corollary 2.6, which states

> Suppose there is a b in Z_n such that the equation
>
> $$a \cdot_n x = b$$
>
> does not have a solution. Then a does not have a multiplicative inverse in Z_n.

We had assumed that the hypothesis of the corollary was true so that $a \cdot_n x = b$ does not have a solution. Then we assumed the conclusion that a does not have a multiplicative inverse was false. We saw that these two assumptions led to a contradiction, so that it was impossible for both of them to be true. Thus we concluded whenever the first assumption was true, the second had to be false. Why could we conclude this? Because the principle of the excluded middle says that the second assumption has to be either true or false. We didn't introduce the principle of the excluded middle at this point for two reasons. First, we expected that the reader would agree with our proof even if we didn't mention the principle, and second, we didn't want to confuse the reader's understanding of proof by contradiction by talking about two principles at once!

Important Concepts, Formulas, and Theorems

1. *Logical statements.* Logical statements may be built up from the following notation:
   - symbols (s, t, etc.) standing for statements (these will be called *variables*),
   - the symbol $\wedge$, standing for "and,"
   - the symbol $\vee$, standing for "or,"
   - the symbol $\oplus$ standing for "exclusive or,"
   - the symbol $\neg$, standing for "not,"

- the symbol $\Rightarrow$, standing for "implies," and
- the symbol $\Leftrightarrow$, standing for "if and only if."

The operators $\wedge$, $\vee$, $\oplus$, $\Rightarrow$, $\Leftrightarrow$, and $\neg$ are called *logical connectives*. The operators $\Rightarrow$ and $\Leftrightarrow$ are called *conditional connectives*.

2. *Truth Tables.* The following are truth tables for the basic logical connectives:

AND

s	t	$s \wedge t$
T	T	T
T	F	F
F	T	F
F	F	F

OR

s	t	$s \vee t$
T	T	T
T	F	T
F	T	T
F	F	F

XOR

s	t	$s \oplus t$
T	T	F
T	F	T
F	T	T
F	F	F

NOT

s	$s \oplus t$
T	F
F	T

3. *Equivalence of logical statements.* We say that two symbolic compound statements are *equivalent* if they are true in exactly the same cases.

4. *Distributive Law.* The statements

$$w \wedge (u \vee v)$$

and

$$(w \wedge u) \vee (w \wedge v)$$

are equivalent.

5. *DeMorgan's Laws.* DeMorgan's Laws say that $\neg(p \vee q)$ is equivalent to $\neg p \wedge \neg q$, and that $\neg(p \wedge q)$ is equivalent to $\neg p \vee \neg q$.

6. *Implication.* The following four English phrases are equivalent:

- s implies t,
- if s then t,
- t if s, and
- s only if t.

7. *Truth tables for implies and if and only if.*

IMPLIES

s	t	$s \Rightarrow t$
T	T	T
T	F	F
F	T	T
F	F	T

IF AND ONLY IF

s	t	$s \Leftrightarrow t$
T	T	T
T	F	F
F	T	F
F	F	T

8. *Principle of the Excluded Middle.* A statement is true exactly when it is not false.

Problems

1. Give truth tables for the following expressions:

   a. $(s \vee t) \wedge (\neg s \vee t) \wedge (s \vee \neg t)$
   b. $(s \Rightarrow t) \wedge (t \Rightarrow u)$
   c. $(s \vee t \vee u) \wedge (s \vee \neg t \vee u)$

2. Find at least two more examples of the use of some word or phrase equivalent to "implies" in lemmas, theorems, or corollaries in Chapters One or Two.

3. Find at least two more examples of the use of the phrase "if and only if" in lemmas, theorems, and corollaries in Chapters One or Two.

4. Show that the statements $s \Rightarrow t$ and $\neg s \vee t$ are equivalent.

5. Prove the DeMorgan law which states $\neg(p \wedge q) = \neg p \vee \neg q$.

6. Show that $p \oplus q$ is equivalent to $(p \wedge \neg q) \vee (\neg p \wedge q)$.

7. Give a simplified form of each of the following expressions (using T to stand for a statement that is always true and F to stand for a statement that is always false)[3]:

   - $s \vee s$,
   - $s \wedge s$,
   - $s \vee \neg s$,
   - $s \wedge \neg s$.

8. Use a truth table to show that $(s \vee t) \wedge (u \vee v)$ is equivalent to $(s \wedge u) \vee (s \wedge v) \vee (t \wedge u) \vee (t \wedge v)$. What algebraic rule is this similar to?

9. Use DeMorgan's Law, the distributive law, and Problems 7 and 8 to show that $\neg((s \vee t) \wedge (s \vee \neg t))$ is equivalent to $\neg s$.

10. Give an example in English where "or" seems to you to mean exclusive or (or where you think it would for many people) and an example in English where "or" seems to you to mean inclusive or (or where you think it would for many people).

11. Give an example in English where "if ... then" seems to you to mean "if and only if" (or where you think it would to many people) and an example in English where it seems to you not to mean "if and only if" (or where you think it would not to many people).

12. Find a statement involving only $\wedge$, $\vee$ and $\neg$ (and s and t) equivalent to $s \Leftrightarrow t$. Does your statement have as few symbols as possible? If you think it doesn't, try to find one with fewer symbols.

13. Suppose that for each line of a 2-variable truth table, you are told whether the final column in that line should evaluate to true or to false. (For example, you might be told that the final column should contain T, F, T, and F in that order.) Explain how to create a logical statement using the symbols s, t, $\wedge$, $\vee$, and $\neg$ that has that pattern as its final column. Can you extend this procedure to an arbitrary number of variables?

[3] A statement that is always true is called a *tautology*; a statement that is always false is called a *contradiction*

14. In Problem 13, your solution may have used $\wedge$, $\vee$ and $\neg$. Is it possible to give a solution using only one of those symbols? Is it possible to give a solution using only two of these symbols?

15. We proved that $\wedge$ distributes over $\vee$ in the sense of giving two equivalent statements that represent the two "sides" of the distributive law. For each question below, explain why your answer is true.

    a. Does $\vee$ distribute over $\wedge$?

    b. Does $\vee$ distribute over $\oplus$?

    c. Does $\wedge$ distribute over $\oplus$?

3.2 Variables and Quantifiers

Variables and universes

Statements we use in computer languages to control loops or conditionals are statements about variables. When we declare these variables, we give the computer information about their possible values. For example, in some programming languages we may declare a variable to be a "boolean" or an "integer" or a "real."[4] In English and in mathematics, we also make statements about variables, but it is not always clear which words are being used as variables and what values these variables may take on. We use the phrase *varies over* to describe the set of values a variable may take on. For example, in English, we might say "If someone's umbrella is up, then it must be raining." In this case, the word "someone" is a variable, and presumably it *varies over* the people who happen to be in a given place at a given time. In mathematics, we might say "For every pair of positive integers m and n, there are nonnegative integers q and r with $0 \leq r < n$ such that $m = nq + r$." In this case m, n, q, and r are clearly our variables; our statement itself suggests that two of our variables range over the positive integers and two range over the nonnegative integers. We call the set of possible values for a variable the *universe* of that variable.

In the statement "m is an even integer," it is clear that m is a variable, but the universe is not given. It might be the integers, just the even integers, or the rational numbers, or one of many other sets. The choice of the universe is crucial for determining the truth or falsity of a statement. If we choose the set of integers as the universe for m, then the statement is true for some integers and false for others. On the other hand, if we choose integer multiples of 10 as our universe, then the statement is always true. In the same way, when we control a while loop with a statement such as "$i < j$" there are some values of i and j for which the statement is true and some for which it is false. In statements like "m is an even integer" and "$i < j$" our variables are not constrained and so are called *free variables.* For each possible value of a free variable, we have a new statement, which might be either true or false, determined by substituting the possible value for the variable. The truth value of the statement is determined only after such a substitution.

Exercise 3.2-1 For what values of m is the statement $m^2 > m$ a true statement and for what values is it a false statement? Since we have not specified a universe, your answer will depend on what universe you choose to use.

If you used the universe of positive integers, the statement is true for every value of m but 1; if you used the real numbers, the statement is true for every value of m except for those in the closed interval $[0, 1]$. There are really two points to make here. First, a statement about a variable can often be interpreted as a statement about more than one universe, and so to make it unambiguous, the universe must be clearly stated. Second, a statement about a variable can be true for some values of a variable and false for others.

[4]Note that to declare a variable x as an integer in, say, a C program does not mean that same thing as saying that x is an integer. In a C program, an integer may really be a 32-bit integer, and so it is limited to values between $2^{31} - 1$ and -2^{31}. Similarly a real has some fixed precision, and hence a real variable y may not be able to take on a value of, say, 10^{-985}.

Quantifiers

In contrast, the statement

$$\text{For every integer } m,\ m^2 > m. \tag{3.1}$$

is false; we do not need to qualify our answer by saying that it is true some of the time and false at other times. To determine whether Statement 3.1 is true or false, we could substitute various values for m into the simpler statement $m^2 > m$, and decide, for each of these values, whether the statement $m^2 > m$ is true or false. Doing so, we see that the statement $m^2 > m$ is true for values such as $m = -3$ or $m = 9$, but false for $m = 0$ or $m = 1$. Thus it is not the case that for every integer m, $m^2 > m$, so Statement 3.1 is false. It is false as a statement because it is an assertion that the simpler statement $m^2 > m$ holds for each integer value of m we substitute in. A phrase like "for every integer m" that converts a symbolic statement about potentially any member of our universe into a statement about the universe instead is called a *quantifier*. A quantifier that asserts a statement about a variable is true for every value of the variable in its universe is called a *universal quantifier.*

The previous example illustrates a very important point.

> If a statement asserts something for every value of a variable, then to show the statement is false, we need only give one value of the variable for which the assertion is untrue.

Another example of a quantifier is the phrase "There is an integer m" in the sentence

> There is an integer m such that $m^2 > m$.

This statement is also about the universe of integers, and as such it is true—there are plenty of integers m we can substitute into the symbolic statement $m^2 > m$ to make it true. This is an example of an "existential quantifier." An *existential quantifier* asserts that a certain element of our universe exists. A second important point similar to the one we made above is:

> To show that a statement with an existential quantifier is *true*, we need only exhibit one value of the variable being quantified that makes the statement true.

As the more complex statement

> For every pair of positive integers m and n, there are nonnegative integers q and r with $0 \leq r < n$ such that $m = qn + r$,

shows, statements of mathematical interest abound with quantifiers. Recall the following definition of the "big-O" notation you have probably used in earlier computer science courses:

Definition 3.2 *We say that $f(x) = O(g(x))$ if there are positive numbers c and n_0 such that $f(x) \leq cg(x)$ for every $x > n_0$.*

Exercise 3.2-2 Quantification is present in our everyday language as well. The sentences "Every child wants a pony" and "No child wants a toothache" are two different examples of quantified sentences. Give ten examples of everyday sentences that use quantifiers, but use different words to indicate the quantification.

Exercise 3.2-3 Convert the sentence "No child wants a toothache" into a sentence of the form "It is not the case that..." Find an existential quantifier in your sentence.

Exercise 3.2-4 What would you have to do to show that a statement about one variable with an existential quantifier is *false*? Correspondingly, what would you have to do to show that a statement about one variable with a universal quantifier is *true*?

As Exercise 3.2-2 points out, English has many different ways to express quantifiers. For example, the sentences, "All hammers are tools", "Each sandwich is delicious", "No one in their right mind would do that", "Somebody loves me", and "Yes Virginia, there is a Santa Claus" all contain quantifiers. For Exercise 3.2-3, we can say "It is not the case that there is a child who wants a toothache." Our quantifier is the phrase "there is."

To show that a statement about one variable with an existential quantifier is false, we have to show that every element of the universe makes the statement (such as $m^2 > m$) false. Thus to show that the statement "There is an x in $[0, 1]$ with $x^2 > x$" is false, we have to show that every x in the interval makes the statement $x^2 > x$ false. Similarly, to show that a statement with a universal quantifier is true, we have to show that the statement being quantified is true for every member of our universe. We will give more details about how to show a statement about a variable is true or false for every member of our universe later in this section.

Mathematical statements of theorems, lemmas, and corollaries often have quantifiers. For example in Lemma 2.5 the phrase "for any" is a quantifier, and in Corollary 2.6 the phrase "there is" is a quantifier.

Standard notation for quantification

Each of the many variants of language that describe quantification describe one of two situations:

A quantified statement about a variable x asserts either

- that the statement is true for all x in the universe, or
- that there exists an x in the universe that makes the statement true.

All quantified statements have one of these two forms. We use the standard shorthand of $\forall$ for the phrase "for all" and the standard shorthand of $\exists$ for the phrase "there exists." We also adopt the convention that we parenthesize the expression that is subject to the quantification. For example, using Z to stand for the universe of all integers, we write

$$\forall n \in Z \; (n^2 \geq n)$$

as a shorthand for the statement "For all integers n, $n^2 \geq n$." It is perhaps more natural to read the notation as "For all n in Z, $n^2 \geq n$," which is how we recommend reading the symbolism. We similarly use

$$\exists n \in Z(n^2 \not> n)$$

to stand for "There exists an n in Z such that $n^2 \not> n$." Notice that in order to cast our symbolic form of an existence statement into grammatical English we have included the supplementary word "an" and the supplementary phrase "such that." People often leave out the "an" as they read an existence statement, but rarely leave out the "such that." Such supplementary language is not needed with $\forall$.

As another example, we rewrite the definition of the "Big Oh" notation with these symbols. We use the letter R to stand for the universe of real numbers, and the symbol R^+ to stand for the universe of positive real numbers.

$$f = O(g) \text{ means that } \exists c \in R^+(\exists n_0 \in R^+(\forall x \in R(x > n_0 \Rightarrow f(x) \leq cg(x))))$$

We would read this literally as

> f is big Oh of g means that there exists a c in R^+ such that there exists an n_0 in R^+ such that for all x in R, if $x > n_0$, then $f(x) \leq cg(x)$.

Clearly this has the same meaning (when we translate it into more idiomatic English) as

> f is big Oh of g means that there exist a c in R^+ and an n_0 in R^+ such that for all real numbers $x > n_0$, $f(x) \leq cg(x)$.

This statement is identical to the definition of "big Oh" that we gave earlier in Definition 3.2, except for more precision as to what c and n_0 actually are.

Exercise 3.2-5 How would you rewrite Euclid's division theorem, Theorem 2.12 using the shorthand notation we have introduced for quantifiers? Use Z^+ to to stand for the positive integers and N to stand for the nonnegative integers.

We can rewrite Euclid's division theorem as

$$\forall m \in N(\forall n \in Z^+(\exists q \in N(\exists r \in N((r < n) \wedge (m = qn + r))))).$$

Statements about variables

To talk about statements about variables, we need a notation to use for such statements. For example, we can use $p(n)$ to stand for the statement $n^2 > n$. Now, we can say that $p(4)$ and $p(-3)$ are true, while $p(1)$ and $p(.5)$ are false. In effect we are introducing variables that stand for statements about (other) variables! We typically use symbols like $p(n)$, $q(x)$, etc. to stand for statements about a variable n or x. Then the statement "For all x in U $p(x)$" can be written as $\forall x \in U(p(x))$ and the statement "There exists an n in U such that $q(n)$" can be written as $\exists n \in U(q(n))$. Sometimes we have statements about more than one variable; for example, our definition of "big Oh" notation had the form $\exists c(\exists n_0(\forall x(p(c, n_0, x))))$, where $p(c, n_0, x)$ is $(x > n_0 \Rightarrow f(x) \leq cg(x))$. (We have left out mention of the universes for our variables here to emphasize the form of the statement.)

Exercise 3.2-6 Rewrite Euclid's division theorem, using the notation above for statements about variables. Leave out the references to universes so that you can see clearly the order in which the quantifiers occur.

The form of Euclid's division theorem is $\forall m(\forall n(\exists q(\exists r(p(m, n, q, r)))))$.

Rewriting statements to encompass larger universes

It is sometimes useful to rewrite a quantified statement so that the universe is larger, and the statement itself serves to limit the scope of the universe.

Exercise 3.2-7 Let R to stand for the real numbers and R^+ to stand for the positive real numbers. Consider the following two statements:

a) $\forall x \in R^+(x > 1)$

b) $\exists x \in R^+(x > 1)$

Rewrite these statements so that the universe is all the real numbers, but the statements say the same thing in everyday English that they did before.

For Exercise 3.2-7, there are potentially many ways to rewrite the statements. Two particularly simple ways are $\forall x \in R(x > 0 \Rightarrow x > 1)$ and $\exists x \in R(x > 0 \wedge x > 1)$. Notice that we translated one of these statements with "implies" and one with "and." We can state this rule as a general theorem:

Theorem 3.2 *Let U_1 be a universe, and let U_2 be another universe with $U_1 \subseteq U_2$. Suppose that $q(x)$ is a statement such that*

$$U_1 = \{x|\ q(x) \text{ is true}\}. \tag{3.2}$$

Then if $p(x)$ is a statement about U_2, it may also be interpreted as a statement about U_1, and

(a) $\forall x \in U_1(p(x))$ *is equivalent to* $\forall x \in U_2(q(x) \Rightarrow p(x))$.

(b) $\exists x \in U_1(p(x))$ *is equivalent to* $\exists x \in U_2(q(x) \wedge p(x))$.

Proof: By Equation 3.2 the statement $q(x)$ must be true for all $x \in U_1$ and false for all x in U_2 but not U_1. To prove part (a) we must show that $\forall x \in U_1(p(x))$ is true in exactly the same cases as the statement $\forall x \in U_2(q(x) \Rightarrow p(x))$. For this purpose, suppose first that $\forall x \in U_1(p(x))$ is true. Then $p(x)$ is true for all x in U_1. Therefore, by the truth table for "implies" and our remark about Equation 3.2, the statement $\forall x \in U_2(q(x) \Rightarrow p(x))$ is true. Now suppose $\forall x \in U_1(p(x))$ is false. Then there exists an x in U_1 such that $p(x)$ is false. Then by the truth table for "implies," the statement $\forall x \in U_2(q(x) \Rightarrow p(x))$ is false. Thus the statement $\forall x \in U_1(p(x))$ is true if and only if the statement $\forall x \in U_2(q(x) \Rightarrow p(x))$ is true. Therefore the two statements are true in exactly the same cases. Part (a) of the theorem follows.

Similarly, for Part (b), we observe that if $\exists x \in U_1(p(x))$ is true, then for some $x' \in U_1$, $p(x')$ is true. For that x', $q(x')$ is also true, and hence $p(x') \wedge q(x')$ is true, so that $\exists x \in U_2(q(x) \wedge p(x))$ is true as well. On the other hand, if $\exists x \in U_1(p(x))$ is false, then no $x \in U_1$ has $p(x)$ true. Therefore by the truth table for "and" $q(x) \wedge p(x)$ won't be true either. Thus the two statements in Part (b) are true in exactly the same cases and so are equivalent. ■

Proving quantified statements true or false

Exercise 3.2-8 Let R stand for the real numbers and R^+ stand for the positive real numbers. For each of the following statements, say whether it is true or false and why.

a) $\forall x \in R^+(x > 1)$
b) $\exists x \in R^+(x > 1)$
c) $\forall x \in R(\exists y \in R(y > x))$
d) $\forall x \in R(\forall y \in R(y > x))$
e) $\exists x \in R(x \geq 0 \wedge \forall y \in R^+(y > x))$

In Exercise 3.2-8, since .5 is not greater than 1, statement (a) is false. However since $2 > 1$, statement (b) is true. Statement (c) says that for each real number x there is a real number y bigger than x, which we know is true. Statement (d) says that every y in R is larger than every x in R, and so it is false. Statement (e) says that there is a nonnegative number x such that every positive y is larger than x, which is true because $x = 0$ fills the bill.

We can summarize what we know about the meaning of quantified statements as follows.

Principle 3.2 (The meaning of quantified statements)

- *The statement $\exists x \in U(p(x))$ is true if there is at least one value of x in U for which the statement $p(x)$ is true.*
- *The statement $\exists x \in U(p(x))$ is false if there is no $x \in U$ for which $p(x)$ is true.*
- *The statement $\forall x \in U(p(x))$ is true if $p(x)$ is true for each value of x in U.*
- *The statement $\forall x \in U(p(x))$ is false if $p(x)$ is false for at least one value of x in U.*

Negation of quantified statements

An interesting connection between $\forall$ and $\exists$ arises from the negation of statements.

Exercise 3.2-9 What does the statement "It is not the case that for all integers n, $n^2 > 0$" mean?

From our knowledge of English we see that since the statement $\neg\forall n \in Z(n^2 > 0)$ asserts that it is not the case that, for all integers n, we have $n^2 > 0$, there must be some integer n such that $n^2 \not> 0$. In other words, it says there is some integer n such that $n^2 \leq 0$. Thus the negation of our "for all" statement is a "there exists" statement. We can make this idea more precise by recalling the notion of equivalence of statements. We have said that two symbolic statements are *equivalent* if they are true in exactly the same cases. By considering the case when $p(x)$ is true for all $x \in U$, (we call this case "always true") and the case when $p(x)$ is false for at least one $x \in U$ (we call this case "not always true") we can analyze the equivalence. The theorem that follows, which formalizes the example above in which $p(x)$ was the statement $x^2 > 0$, is proved by dividing these cases into two possibilities.

Theorem 3.3 *The statements* $\neg\forall x \in U(p(x))$ *and* $\exists x \in U(\neg p(x))$ *are equivalent.*

Proof: Consider the following table which we have set up much like a truth table, except that the relevant cases are not determined by whether $p(x)$ is true or false, but by whether $p(x)$ is true for all x in the universe U or not.

$p(x)$	$\neg p(x)$	$\forall x \in U(p(x))$	$\neg\forall x \in U(p(x))$	$\exists x \in U(\neg p(x))$
always true	always false	true	false	false
not always true	not always false	false	true	true

Since the last two columns are identical, the theorem holds. ■

Corollary 3.4 *The statements* $\neg\exists x \in U(q(x))$ *and* $\forall x \in U(\neg q(x))$ *are equivalent.*

Proof: Since the two statements in Theorem 3.3 are equivalent, their negations are also equivalent. We then substitute $\neg q(x)$ for $p(x)$ to prove the corollary. ■

Put another way, to negate a quantified statement, you switch the quantifier and "push" the negation inside.

To deal with the negation of more complicated statements, we simply take them one quantifier at a time. Recall Definition 3.2, the definition of big Oh notation,

$$f(x) = O(g(x)) \text{ if } \exists c \in R^+(\exists n_0 \in R^+(\forall x \in R(x > n_0 \Rightarrow f(x) \leq cg(x)))).$$

What does it mean to say that $f(x)$ is *not* $O(g(x))$? First we can write

$$f(x) \neq O(g(x)) \text{ if } \neg\exists c \in R^+(\exists n_0 \in R^+(\forall x \in R(x > n_0 \Rightarrow f(x) \leq cg(x)))).$$

After one application of Corollary 3.4 we get

$$f(x) \neq O(g(x)) \text{ if } \forall c \in R^+(\neg\exists n_0 \in R^+(\forall x \in R(x > n_0 \Rightarrow f(x) \leq cg(x)))).$$

After another application of Corollary 3.4 we obtain

$$f(x) \neq O(g(x)) \text{ if } \forall c \in R^+(\forall n_0 \in R^+(\neg\forall x \in R(x > n_0 \Rightarrow f(x) \leq cg(x)))).$$

Now we apply Theorem 3.3 and obtain

$$f(x) \neq O(g(x)) \text{ if } \forall c \in R^+(\forall n_0 \in R^+(\exists x \in R(\neg(x > n_0 \Rightarrow f(x) \leq cg(x))))).$$

Now $\neg(p \Rightarrow q)$ is equivalent to $p \wedge \neg q$, so we can write

$$f(x) \neq O(g(x)) \text{ if } \forall c \in R^+(\forall n_0 \in R^+(\exists x \in R((x > n_0) \wedge (f(x) \not\leq cg(x))))).$$

Thus $f(x)$ is *not* $O(g(x))$ if for every c in $R+$ and every n_0 in R^+, there is an x such that $x > n_0$ and $f(x) \not\leq cg(x)$.

In our next exercise, we use the "Big Theta" notation defined as follows:

Definition 3.3 *$f(x) = \Theta(g(x))$ means that $f(x) = O(g(x))$* **and** *$g(x) = O(f(x))$.*

Exercise 3.2-10 Express $\neg(f(x) = \Theta(g(x)))$ in terms similar to those we used to describe $f(x) \neq O(g(x))$.

Exercise 3.2-11 Suppose the universe for a statement $p(x)$ is the integers from 1 to 10. Express the statement $\forall x(p(x))$ without any quantifiers. Express the negation in terms of $\neg p$ without any quantifiers. Discuss how negation of "for all" and "there exists" statements corresponds to DeMorgan's Law.

By DeMorgan's law, $\neg(f = \Theta(g))$ means $\neg(f = O(g)) \vee \neg(g = O(f))$. Thus $\neg(f = \Theta(g))$ means that either for every c and n_0 in R^+ there is an x in R with $x > n_0$ and $f(x) \not< cg(x)$ or for every c and n_0 in R^+ there is an x in R with $x > n_0$ and $g(x) < cf(x)$ (or both).

For Exercise 3.2-11 we see that $\forall x(p(x))$ is simply

$$p(1) \wedge p(2) \wedge p(3) \wedge p(4) \wedge p(5) \wedge p(6) \wedge p(7) \wedge p(8) \wedge p(9) \wedge p(10).$$

By DeMorgan's law the negation of this statement is

$$\neg p(1) \vee \neg p(2) \vee \neg p(3) \vee \neg p(4) \vee \neg p(5) \vee \neg p(6) \vee \neg p(7) \vee \neg p(8) \vee \neg p(9) \vee \neg p(10).$$

Thus the relationship that negation gives between "for all" and "there exists" statements is the extension of DeMorgan's law from a finite number of statements to potentially infinitely many statements about a potentially infinite universe.

Implicit quantification

Exercise 3.2-12 Are there any quantifiers in the statement "The sum of even integers is even?"

It is an elementary fact about numbers that the sum of even integers is even. Another way to say this is that if m and n are even, then $m + n$ is even. If $p(n)$ stands for the statement "n is even," then this last sentence translates to $p(m) \wedge p(n) \Rightarrow p(m + n)$. From the logical form of the statement, we see that our variables are free, so we could substitute various integers in for m and n to see whether the statement is true. But in Exercise 3.2-12, we said we were stating a more general fact about the integers. What we meant to say is that for *every pair of integers m* and n, if m and n are even, then $m + n$ is even. In symbols, using $p(k)$ for "k is even," we have

$$\forall m \in Z(\forall n \in Z(p(m) \wedge p(n) \Rightarrow p(m + n))).$$

This way of representing the statement captures the meaning we originally intended. This is one of the reasons that mathematical statements and their proofs sometimes seem confusing—just as in English, sentences in mathematics have to be interpreted in context. Since mathematics has to be written in some natural language, and since context is used to remove ambiguity in natural language, so must context be used to remove ambiguity from mathematical statements made in natural language. In fact, we frequently rely on context in writing mathematical statements with implicit quantifiers because, in context, it makes the statements easier to read. For example, in Lemma 2.8 we said

> The equation
> $$a \cdot_n x = 1$$
> has a solution in Z_n if and only if there exist integers x and y such that
> $$ax + ny = 1.$$

In context it was clear that the a we were talking about was an arbitrary member of Z_n. It would simply have made the statement read more clumsily if we had said

> For every $a \in Z_n$, the equation
> $$a \cdot_n x = 1$$
> has a solution in Z_n if and only if there exist integers x and y such that
> $$ax + ny = 1.$$

On the other hand, we were making a transition from talking about Z_n to talking about the integers, so it was important for us to include the quantified statement "there exist integers x and y such that $ax+ny = 1$." More recently in Theorem 3.3, we also did not feel it was necessary to say "For all universes U and for all statements p about U," at the beginning of the theorem. We felt the theorem would be easier to read if we kept those quantifiers implicit and let the reader (not necessarily consciously) infer them from context.

Proof of quantified statements

We said that "the sum of even integers is even" is an elementary fact about numbers. How do we know it is a fact? One answer is that we know it because our teachers told us so. (And presumably they knew it because their teachers told them so.) But someone had to figure it out in the first place, and so we ask how we would prove this statement? A mathematician asked to give a proof that the sum of even numbers is even might write

> If m and n are even, then $m = 2i$ and $n = 2j$ so that
> $$m + n = 2i + 2j = 2(i + j)$$
> and thus $m + n$ is even.

Because mathematicians think and write in natural language, they will often rely on context to remove ambiguities. For example, there are no quantifiers in the proof above. However the sentence, while technically incomplete as a proof, captures the essence of why the sum of two even numbers is even. A typical complete (but more formal and wordy than usual) proof might go like this.

> Let m and n be integers. Suppose m and n are even. If m and n are even, then by definition there are integers i and j such that $m = 2i$ and $n = 2j$. Thus there are integers i and j such that $m = 2i$ and $n = 2j$. Then
> $$m + n = 2i + 2j = 2(i + j),$$
> so by definition $m + n$ is an even integer. We have shown that if m and n are even, then $m + n$ is even. Therefore for every m and n, if m and n are even integers, then so is $m + n$.

We began our proof by assuming that m and n are integers. This gives us symbolic notation for talking about two integers. We then appealed to the definition of an even integer, namely that an integer h is even if there is another integer k so that $h = 2k$. (Note the use of a quantifier in the definition.) Then we used algebra to show that $m + n$ is also two times another number. Since this is the definition of $m + n$ being even, we concluded that $m + n$ is even. This allowed us to say that if m and n are even, the $m + n$ is even. Then we asserted that for every pair of integers m and n, if m and n are even, then $m + n$ is even.

There are a number of principles of proof illustrated here. The next section will be devoted to a discussion of principles we use in constructing proofs. For now, let us conclude with a remark about the limitations of logic. How did we know that we wanted to write the symbolic equation

$$m + n = 2i + 2j = 2(i + j)?$$

It was not logic that told us to do this, but intuition and experience.

Important Concepts, Formulas, and Theorems

1. *Varies over.* We use the phrase *varies over* to describe the set of values a variable may take on.

2. *Universe.* We call the set of possible values for a variable the *universe* of that variable.

3. *Free variables.* Variables that are not constrained in any way whatever are called *free variables.*

4. *Quantifier.* A phrase that converts a symbolic statement about potentially any member of our universe into a statement about the universe instead is called a *quantifier.* There are two types of quantifiers:

   - *Universal quantifier.* A quantifier that asserts a statement about a variable is true for every value of the variable in its universe is called a *universal quantifier.*
   - *Existential quantifier.* A quantifier that asserts a statement about a variable is true for at least one value of the variable in its universe is called an *existential quantifier.*

5. *Larger universes.* Let U_1 be a universe, and let U_2 be another universe with $U_1 \subseteq U_2$. Suppose that $q(x)$ is a statement such that

   $$U_1 = \{x|\ q(x) \text{ is true}\}.$$

   Then if $p(x)$ is a statement about U_2, it may also be interpreted as a statement about U_1, and

   (a) $\forall x \in U_1(p(x))$ is equivalent to $\forall x \in U_2(q(x) \Rightarrow p(x))$.
   (b) $\exists x \in U_1(p(x))$ is equivalent to $\exists x \in U_2(q(x) \wedge p(x))$.

6. *Proving quantified statements true or false.*

   - The statement $\exists x \in U(p(x))$ is true if there is at least one value of x in U for which the statement $p(x)$ is true.

- The statement $\exists x \in U(p(x))$ is false if there is no $x \in U$ for which $p(x)$ is true.
- The statement $\forall x \in U(p(x))$ is true if $p(x)$ is true for each value of x in U.
- The statement $\forall x \in U(p(x))$ is false if $p(x)$ is false for at least one value of x in U.

7. *Negation of quantified statements.* To negate a quantified statement, you switch the quantifier and push the negation inside.
   - The statements $\neg\forall x \in$U$(p(x))$ and $\exists x \in U(\neg p(x))$ are equivalent.
   - The statements $\neg\exists x \in$U$(p(x))$ and $\forall x \in U(\neg p(x))$ are equivalent.
8. *Big-Oh* We say that $f(x) = O(g(x))$ if there are positive numbers c and n_0 such that $f(x) \leq cg(x)$ for every $x > n_0$.
9. *Big-Theta.* $f(x) = \Theta(g(x))$ means that $f = O(g(x))$ **and** $g = O(f(x))$.
10. *Some notation for sets of numbers.* We use R to stand for the real numbers, R^+ to stand for the positive real numbers, Z to stand for the integers (positive, negative, and zero), Z^+ to stand for the positive integers, and N to stand for the nonnegative integers.

Problems

1. For what positive integers x is the statement $(x-2)^2+1 \leq 2$ true? For what integers is it true? For what real numbers is it true? If we expand the universe for which we are considering a statement about a variable, does this always increase the size of the statement's truth set?
2. Is the statement "There is an integer greater than 2 such that $(x-2)^2+1 \leq 2$" true or false? How do you know?
3. Write the statement that the square of every real number is greater than or equal to zero as a quantified statement about the universe of real numbers. You may use R to stand for the universe of real numbers.
4. The definition of a prime number is that it is an integer greater than 1 whose only positive integer factors are itself and 1. Find two ways to write this definition so that all quantifiers are explicit. (It may be convenient to introduce a variable to stand for the number and perhaps a variable or some variables for its factors.)
5. Write down the definition of a greatest common divisor of m and n in such a way that all quantifiers are explicit and expressed explicitly as "for all" or "there exists." Write down Euclid's extended greatest common divisor theorem that relates the greatest common divisor of m and n algebraically to m and n. Again make sure all quantifiers are explicit and expressed explicitly as "for all" or "there exists."
6. What is the form of the definition of a greatest common divisor, using $s(x, y, z)$ to be the statement $x = yz$ and $t(x, y)$ to be the statement $x < y$? (You need not include references to the universes for the variables.)
7. Which of the following statements (in which Z^+ stands for the positive integers and Z stands for all integers) is true and which is false, and why?

(a) $\forall z \in Z^+(z^2 + 6z + 10 > 20)$.
(b) $\forall z \in Z(z^2 - z \geq 0)$.
(c) $\exists z \in Z^+(z - z^2 > 0)$.
(d) $\exists z \in Z(z^2 - z = 6)$.

8. Are there any (implicit) quantifiers in the statement "The product of odd integers is odd?" If so, what are they?

9. Rewrite the statement "The product of odd integers is odd," with all quantifiers (including any in the definition of odd integers) explicitly stated as "for all" or "there exist."

10. Rewrite the following statement without any negations. It is not the case that there exists an integer n such that $n > 0$ and for all integers $m > n$, for every polynomial equation $p(x) = 0$ of degree m there are no real numbers for solutions.

11. Consider the following slight modification of Theorem 3.2. For each part below, either prove that it is true or give a counterexample.

    Let U_1 be a universe, and let U_2 be another universe with $U_1 \subseteq U_2$. Suppose that $q(x)$ is a statement such that $U_1 = \{x|\ q(x) \text{ is true}\}$.

    (a) $\forall x \in U_1(p(x))$ is equivalent to $\forall x \in U_2(q(x) \wedge p(x))$.
    (b) $\exists x \in U_1(p(x))$ is equivalent to $\exists x \in U_2(q(x) \Rightarrow p(x))$.

12. Let $p(x)$ stand for "x is a prime," $q(x)$ for "x is even," and $r(x, y)$ stand for "$x = y$." Write down the statement "There is one and only one even prime," using these three symbolic statements and appropriate logical notation. (Use the set of integers for your universe.)

13. Each expression below represents a statement about the integers. Using $p(x)$ for "x is prime," $q(x, y)$ for "$x = y^2$," $r(x, y)$ for "$x \leq y$," $s(x, y, z)$ for "$z = xy$," and $t(x, y)$ for "$x = y$," determine which expressions represent true statements and which represent false statements.

    (a) $\forall x \in Z(\exists y \in Z(q(x, y) \vee p(x)))$
    (b) $\forall x \in Z(\forall y \in Z(s(x, x, y) \Leftrightarrow q(x, y)))$
    (c) $\forall y \in Z(\exists x \in Z(q(y, x)))$
    (d) $\exists z \in Z(\exists x \in Z(\exists y \in Z(p(x) \wedge p(y) \wedge \neg t(x, y)))$

14. Find a reason why $(\exists x \in U(p(x))) \wedge (\exists y \in U(q(y)))$ is not equivalent to $\exists z \in U(p(z) \vee q(z))$. Are the statements $(\exists x \in U(p(x))) \vee (\exists y \in U(q(y)))$ and $\exists z \in U(p(z) \vee q(z))$ equivalent?

15. Give an example (in English) of a statement that has the form $\forall x \in U(\exists y \in V(p(x, y)))$. (The statement can be a mathematical statement or a statement about "everyday life," or whatever you prefer.) Now write in English the statement using the same $p(x, y)$ but of the form $\exists y \in V(\forall x \in U(p(x, y)))$. Comment on whether "for all" and "there exist" commute.

3.3 Inference

Direct Inference (Modus Ponens) and Proofs

We concluded our last section with a proof that the sum of two even numbers is even. That proof contained several crucial ingredients. First, we introduced symbols for members of the universe of integers. In other words, rather than saying "suppose we have two integers," we introduced symbols for the two members of our universe we assumed we had. How did we know to use algebraic symbols? There are many possible answers to this question, but in this case our intuition was probably based on thinking about what an even number is, and realizing that the definition itself is essentially symbolic. (You may argue that an even number is just twice another number, and you would be right. Apparently no symbols are in that definition. But they really are there; they are the phrases "even number" and "another number." Since we all know algebra is easier with symbolic variables rather than words, we should recognize that it makes sense to use algebraic notation.) Thus this decision was based on experience, not logic.

Next we assumed the two integers were even. We then used the definition of even numbers, and, as our previous parenthetic comment suggests, it was natural to use the definition symbolically. The definition tells us that if m is an even number, then there exists another integer i such that $m = 2i$. We combined this with the assumption that m is even to conclude that in fact there does exist an integer i such that $m = 2i$. This is an example of using the principle of *direct inference* (called *modus ponens* in Latin).

Principle 3.3 (Direct inference) *From p and $p \Rightarrow q$ we may conclude q.*

This common-sense principle is a cornerstone of logical arguments. But why is it true? In Table 3.5 we take another look at the truth table for implication.

Table 3.5: Another look at implication

p	q	$p \Rightarrow q$
T	T	T
T	F	F
F	T	T
F	F	T

The only line which has a T in both the p column and the $p \Rightarrow q$ column is the first line. In this line q is true also, and we therefore conclude that if p and $p \Rightarrow q$ hold then q must hold also. While this may seem like a somewhat "inside out" application of the truth table, it is simply a different way of using a truth table.

There are quite a few rules (called rules of inference) like the principle of direct inference that people commonly use in proofs without explicitly stating them. Before beginning a formal study of rules of inference, we complete our analysis of which rules we used in the proof that the sum of two even integers is even. After concluding that $m = 2i$ and $n = 2j$, we next used algebra to show that because $m = 2i$ and $n = 2j$, there exists a k such that $m + n = 2k$ (our k was $i + j$). Next we used the definition of even number again to say that $m + n$ was even. We then used a rule of inference which says

Principle 3.4 (Conditional Proof) *If, by assuming p, we may prove q, then the statement $p \Rightarrow q$ is true.*

Using this principle, we reached the conclusion that if m and n are even integers, then $m + n$ is an even integer. In order to conclude that this statement is true for all integers m and n, we used another rule of inference, one of the more difficult to describe. We originally introduced the variables m and n. We used only well-known consequences of the fact that they were in the universe of integers in our proof. Thus we felt justified in asserting that what we concluded about m and n is true for any pair of integers. We might say that we were treating m and n as generic members of our universe. Thus our rule of inference says

Principle 3.5 (Universal Generalization) *If we can prove a statement about x by assuming x is a member of our universe, then we can conclude the statement is true for every member of our universe.*

Perhaps the reason this rule is hard to put into words is that it is not simply a description of a truth table, but is a principle that we use in order to prove universally quantified statements.

Rules of inference for direct proofs

We have seen the ingredients of a typical proof. What do we mean by a proof in general? A proof of a statement is a convincing argument that the statement is true. To be more precise about it, we can agree that a *direct proof* consists of a sequence of statements, each of which is either a hypothesis[5], a generally accepted fact, or the result of one of the following rules of inference for compound statements.

Rules of Inference for Direct Proofs

1) From an example x that does not satisfy $p(x)$, we may conclude $\neg p(x)$.

2) From $p(x)$ and $q(x)$, we may conclude $p(x) \wedge q(x)$.

3) From either $p(x)$ or $q(x)$, we may conclude $p(x) \vee q(x)$.

4) From either $q(x)$ or $\neg p(x)$ we may conclude $p(x) \Rightarrow q(x)$.

5) From $p(x) \Rightarrow q(x)$ and $q(x) \Rightarrow p(x)$ we may conclude $p(x) \Leftrightarrow q(x)$.

6) From $p(x)$ and $p(x) \Rightarrow q(x)$ we may conclude $q(x)$.

7) From $p(x) \Rightarrow q(x)$ and $q(x) \Rightarrow r(x)$ we may conclude $p(x) \Rightarrow r(x)$.

8) If we can derive $q(x)$ from the hypothesis that x satisfies $p(x)$, then we may conclude $p(x) \Rightarrow q(x)$.

9) If we can derive $p(x)$ from the hypothesis that x is a (generic) member of our universe U, we may conclude $\forall x \in U(p(x))$.

[5]If we are proving an implication $s \Rightarrow t$, we call s a hypothesis. If we make assumptions by saying "Let ...," "Suppose ...," or something similar before we give the statement to be proved, then these assumptions are hypotheses as well.

10) From an example of an $x \in U$ satisfying $p(x)$ we may conclude $\exists x \in U(p(x))$.

The first rule is a statement of the principle of the excluded middle as it applies to statements about variables. The next four four rules are in effect a description of the truth tables for "and," "or," "implies" and "if and only if." Rule 5 says what we must do in order to write a proof of an "if and only if" statement. Rule 6, exemplified in our earlier discussion, is the principle of direct inference, and describes one row of the truth table for $p \Rightarrow q$. Rule 7 is the transitive law, one we could derive by truth table analysis. Rule 8, the principle of conditional proof, which is also exemplified earlier, may be regarded as yet another description of one row of the truth table of $p \Rightarrow q$. Rule 9 is the principle of universal generalization, discussed and exemplified earlier. Rule 10 specifies what we mean by the truth of an existentially quantified statement, according to Principle 3.2.

Although some of our rules of inference are redundant, they are useful. For example, we could have written a portion of our proof that the sum of even numbers is even as follows without using Rule 8.

> "Let m and n be integers. If m is even, then there is a k with $m = 2k$. If n is even, then there is a j with $n = 2j$. Thus if m is even and n is even, there are a k and j such that $m + n = 2k + 2j = 2(k + j)$. Thus if m is even and n is even, there is an integer $h = k + j$ such that $m + n = 2h$. Thus if m is even and n is even, $m + n$ is even."

This kind of argument could always be used to circumvent the use of Rule 8, so Rule 8 is not required as a rule of inference, but because it permits us to avoid such unnecessarily complicated "silliness" in our proofs, we choose to include it. Rule 7, the transitive law, has a similar role.

Exercise 3.3-1 Prove that if m is even, then m^2 is even. Explain which steps of the proof use one of the rules of inference above.

For Exercise 3.3-1, we can mimic the proof that the sum of even integers is even.

> Let m be integer. Suppose that m is even. If m is even, then there is a k with $m = 2k$. Thus, there is a k such that $m^2 = 4k^2$. Therefore, there is an integer $h = 2k^2$ such that $m^2 = 2h$. Thus if m is even, m^2 is even. Therefore, for all integers m, if m is even, then m^2 is even.

In our first sentence we are setting things up to use Rule 9. In the second sentence we are simply stating an implicit hypothesis. In the next two sentences we use Rule 6, the principle of direct inference. When we said "Therefore, there is an integer $h = 2k^2$ such that $m^2 = 2h$," we were simply stating an algebraic fact. In our next sentence we used Rule 8. Finally, we used Rule 9. You might have written the proof in a different way and used different rules of inference.

Contrapositive rule of inference.

Exercise 3.3-2 Show that "p implies q" is equivalent to "$\neg q$ implies $\neg p$."

Exercise 3.3-3 Is "p implies q" equivalent to "q implies p?"

To do Exercise 3.3-2, we construct the double truth table in Table 3.6. Since the columns under $p \Rightarrow q$ and under $\neg q \Rightarrow \neg p$ are exactly the same, we know the two statements are equivalent. This exercise tells us that if we know that $\neg q \Rightarrow \neg p$, then we can conclude that $p \Rightarrow q$. This is called the *principle of proof by contraposition.*

Table 3.6: A double truth table for $p \Rightarrow q$ and $\neg q \Rightarrow \neg p$.

p	q	$p \Rightarrow q$	$\neg p$	$\neg q$	$\neg q \Rightarrow \neg p$
T	T	T	F	F	T
T	F	F	F	T	F
F	T	T	T	F	T
F	F	T	T	T	T

Principle 3.6 (Proof by Contraposition) *The statement $p \Rightarrow q$ and the statement $\neg q \Rightarrow \neg p$ are equivalent, and so a proof of one is a proof of the other.*

The statement $\neg q \Rightarrow \neg p$ is called the *contrapositive* of the statement $p \Rightarrow q$. The following example demonstrates the utility of the principle of proof by contraposition.

Lemma 3.5 *If n is a positive integer with $n^2 > 100$, then $n > 10$.*

Proof: Suppose n is not greater than 10. (Now we use the rule of algebra for inequalities which says that if $x \leq y$ and $c \geq 0$, then $cx \leq cy$.) Then since $1 \leq n \leq 10$,

$$n \cdot n \leq n \cdot 10 \leq 10 \cdot 10 = 100.$$

Thus n^2 is not greater than 100. Therefore, if n is not greater than 10, n^2 is not greater than 100. Then, by the principle of proof by contraposition, if $n^2 > 100$, n must be greater than 10.■

We adopt Principle 3.6 as a rule of inference, called the *contrapositive* rule of inference.

11) From $\neg q(x) \Rightarrow \neg p(x)$ we may conclude $p(x) \Rightarrow q(x)$.

In our proof of the Chinese Remainder Theorem, Theorem 2.24, we wanted to prove that for a certain function f that if x and y were different integers between 0 and $mn-1$, then $f(x) \neq f(y)$. To prove this we assumed that in fact $f(x) = f(y)$ and proved that x and y were not different integers between 0 and $mn - 1$. Had we known the principle of contrapositive inference, we could have concluded then and there that f was one-to-one. Instead, we used the more common principle of proof by contradiction, the major topic of the remainder of this section, to complete our proof. If you look back at the proof, you will see that we might have been able to shorten it by a sentence by using contrapositive inference.

For Exercise 3.3-3, a quick look at the double truth table for $p \Rightarrow q$ and $q \Rightarrow p$ in Table 3.7 demonstrates that these two statements are *not* equivalent. The statement $q \Rightarrow p$ is called the *converse* of $p \Rightarrow q$. Notice that $p \Leftrightarrow q$ is true exactly when $p \Rightarrow q$ and its converse are true. It is surprising how often people, even professional mathematicians, absent-mindedly try to prove the converse of a statement when they mean to prove the statement itself. Try not to join this crowd!

Table 3.7: A double truth table for $p \Rightarrow q$ and $q \Rightarrow p$.

p	q	$p \Rightarrow q$	$q \Rightarrow p$
T	T	T	T
T	F	F	T
F	T	T	F
F	F	T	T

Proof by contradiction

Proof by contrapositive inference is an example of what we call *indirect proof.* We have actually seen another example indirect proof, the principle of proof by contradiction. In our proof of Corollary 2.6 we introduced the principle of proof by contradiction, Principle 2.1. We were trying to prove the statement

> Suppose there is a b in Z_n such that the equation
>
> $$a \cdot_n x = b$$
>
> does not have a solution. Then a does not have a multiplicative inverse in Z_n.

We assumed that the hypothesis that $a \cdot_n x = b$ does not have a solution was true. We also assumed that the conclusion that a does not have a multiplicative inverse was false. We showed that these two assumptions together led to a contradiction. Then, using the principle of the excluded middle, Principle 3.1 (without saying so), we concluded that if the hypothesis is in fact true, then the only possibility was that the conclusion is true as well.

We used the principle again later in our proof of Euclid's Division Theorem. Recall that in that proof we began by assuming that the theorem was false. We then chose among the pairs of integers (m, n) such that $m \neq qn + r$ with $0 \leq r < n$ a pair with the smallest possible m. We then made some computations by which we proved that in this case there *are* a q and r with $0 \leq r < n$ such that $m = qn + r$. Thus we started out by assuming the theorem was false, and from that assumption we drew drew a contradiction to the assumption. Since all our reasoning, except for the assumption that the theorem was false, used accepted rules of inference, the only source of that contradiction was our assumption. Thus, by the principle of the excluded middle, our assumption had to be incorrect. We adopt the principle of proof by contradiction (also called the principle of *reduction to absurdity*) as our last rule of inference.

12) If from assuming $p(x)$ and $\neg q(x)$, we can derive both $r(x)$ and $\neg r(x)$ for some statement $r(x)$, then we may conclude $p(x) \Rightarrow q(x)$.

There can be many variations of proof by contradiction. For example, we may assume p is true and q is false, and from this derive the contradiction that p is false, as in the following example.

> Prove that if $x^2 + x - 2 = 0$, then $x \neq 0$.
>
> **Proof:** Suppose that $x^2 + x - 2 = 0$. Assume that $x = 0$. Then $x^2 + x - 2 = 0 + 0 - 2 = -2$. This contradicts $x^2 + x - 2 = 0$. Thus (by the principle of proof by contradiction), if $x^2 + x - 2 = 0$, then $x \neq 0$. ■

Here the statement r was identical to p, namely $x^2 + x - 2 = 0$.

On the other hand, we may instead assume p is true and q is false, and derive a contradiction of a known fact, as in the following example.

> Prove that if $x^2 + x - 2 = 0$, then $x \neq 0$.
>
> **Proof:** Suppose that $x^2 + x - 2 = 0$. Assume that $x = 0$. Then $x^2 + x - 2 = 0 + 0 - 2 = -2$. Thus $0 = -2$, a contradiction. Thus (by the principle of proof by contradiction), if $x^2 + x - 2 = 0$, then $x \neq 0$. ■

Here the statement r is the known fact that $0 \neq -2$.

Sometimes the statement r that appears in the principle of proof by contradiction is simply a statement that arises naturally as we are trying to construct our proof, as in the following example.

> Prove that if $x^2 + x - 2 = 0$, then $x \neq 0$.
>
> **Proof:** Suppose that $x^2 + x - 2 = 0$. Then $x^2 + x = 2$. Assume that $x = 0$. Then $x^2 + x = 0 + 0 = 0$. But this is a contradiction (to our observation that $x^2 + x = 2$). Thus (by the principle of proof by contradiction), if $x^2 + x - 2 = 0$, then $x \neq 0$. ■

Here the statement r is "$x^2 + x = 2$."

Finally, if proof by contradiction seems to you not to be much different from proof by contraposition, you are right, as the example that follows shows.

> Prove that if $x^2 + x - 2 = 0$, then $x \neq 0$.
>
> **Proof:** Assume that $x = 0$. Then $x^2+x-2 = 0+0-2 = -2$, so that $x^2+x-2 \neq 0$. Thus (by the principle of proof by contraposition), if $x^2 + x - 2 = 0$, then $x \neq 0$. ■

Any proof that uses one of the indirect methods of inference is called an indirect proof. The last four examples illustrate the rich possibilities that indirect proof provides us. Of course they also illustrate why indirect proof can be confusing. There is no set formula that we use in writing a proof by contradiction, so there is no rule we can memorize in order to formulate indirect proofs. Instead, we have to ask ourselves whether assuming the opposite of what we are trying to prove gives us insight into why the assumption makes no sense. If it does, we have the basis of an indirect proof, and the way in which we choose to write it is a matter of personal choice.

Exercise 3.3-4 Without extracting square roots, prove that if n is a positive integer such that $n^2 < 9$, then $n < 3$. You may use rules of algebra for dealing with inequalities.

Exercise 3.3-5 Prove that $\sqrt{5}$ is not rational.

To prove the statement in Exercise 3.3-4, we assume, for purposes of contradiction, that $n \geq 3$. Squaring both sides of this equation, we obtain

$$n^2 \geq 9 \ ,$$

which contradicts our hypothesis that $n^2 < 9$. Therefore, by the principle of proof by contradiction, $n < 3$.

To prove the statement in Exercise 3.3-5, we assume, for the purpose of contradiction, that $\sqrt{5}$ is rational. This means that it can be expressed as the fraction $\frac{m}{n}$, where m and n are integers. Squaring both sides of the equation $\frac{m}{n} = \sqrt{5}$, we obtain

$$\frac{m^2}{n^2} = 5,$$

or

$$m^2 = 5n^2.$$

Now m^2 must have an even number of prime factors (counting each prime factor as many times as it occurs) as must n^2. But $5n^2$ has an odd number of prime factors. Thus a product of an even number of prime factors is equal to a product of an odd number of prime factors, which is a contradiction since each positive integer may be expressed uniquely as a product of (positive) prime numbers. Thus by the principle of proof by contradiction, $\sqrt{5}$ is not rational.

Important Concepts, Formulas, and Theorems

1. *Principle of direct inference or modus ponens.* From p and $p \Rightarrow q$ we may conclude q.

2. *Principle of conditional proof.* If, by assuming p, we may prove q, then the statement $p \Rightarrow q$ is true.

3. *Principle of universal generalization.* If we can prove a statement about x by assuming x is a member of our universe, then we can conclude it is true for every member of our universe.

4. *Rules of Inference.* 12 rules of inference appear in this chapter. They are

    1) From an example x that does not satisfy $p(x)$, we may conclude $\neg p(x)$.
    2) From $p(x)$ and $q(x)$, we may conclude $p(x) \wedge q(x)$.
    3) From either $p(x)$ or $q(x)$, we may conclude $p(x) \vee q(x)$.
    4) From either $q(x)$ or $\neg p(x)$ we may conclude $p(x) \Rightarrow q(x)$.
    5) From $p(x) \Rightarrow q(x)$ and $q(x) \Rightarrow p(x)$ we may conclude $p(x) \Leftrightarrow q(x)$.
    6) From $p(x)$ and $p(x) \Rightarrow q(x)$ we may conclude $q(x)$.
    7) From $p(x) \Rightarrow q(x)$ and $q(x) \Rightarrow r(x)$ we may conclude $p(x) \Rightarrow r(x)$.
    8) If we can derive $q(x)$ from the hypothesis that x satisfies $p(x)$, then we may conclude $p(x) \Rightarrow q(x)$.
    9) If we can derive $p(x)$ from the hypothesis that x is a (generic) member of our universe U, we may conclude $\forall x \in U(p(x))$.
    10) From an example of an $x \in U$ satisfying $p(x)$ we may conclude $\exists x \in U(p(x))$.
    11) From $\neg q(x) \Rightarrow \neg p(x)$ we may conclude $p(x) \Rightarrow q(x)$.
    12) If from assuming $p(x)$ and $\neg q(x)$, we can derive both $r(x)$ and $\neg r(x)$ for some statement r, then we may conclude $p(x) \Rightarrow q(x)$.

5. *Contrapositive of* $p \Rightarrow q$. The contrapositive of the statement $p \Rightarrow q$ is the statement $\neg q \Rightarrow \neg p$.

6. *Converse of* $p \Rightarrow q$. The converse of the statement $p \Rightarrow q$ is the statement $q \Rightarrow p$.

7. *Contrapositive rule of inference.* From $\neg q \Rightarrow \neg p$ we may conclude $p \Rightarrow q$.

8. *Principle of proof by contradiction.* If from assuming p and $\neg q$, we can derive both r and $\neg r$ for some statement r, then we may conclude $p \Rightarrow q$.

Problems

1. Write down the converse and contrapositive of each of these statements.
   (a) If the hose is 60 feet long, then the hose will reach the tomatoes.
   (b) George goes for a walk only if Mary goes for a walk.
   (c) Pamela recites a poem if Andre asks for a poem.

2. Construct a proof that if m is odd, then m^2 is odd.

3. Construct a proof that for all integers m and n, if m is even and n is odd, then $m + n$ is odd.

4. What do we really mean when we say "prove that if m is odd and n is odd then $m + n$ is even?" Prove this more precise statement.

5. Prove that for all integers m and n if m is odd and n is odd, then $m \cdot n$ is odd.

6. Is the statement $p \Rightarrow q$ equivalent to the statement $\neg p \Rightarrow \neg q$?

7. Construct a contrapositive proof that for all real numbers x if $x^2 - 2x \neq -1$, then $x \neq 1$.

8. Construct a proof by contradiction that for all real numbers x if $x^2 - 2x \neq -1$, then $x \neq 1$.

9. Prove that if $x^3 > 8$, then $x > 2$.

10. Prove that $\sqrt{3}$ is irrational.

11. Construct a proof that if m is an integer such that m^2 is even, then m is even.

12. Prove or disprove the following statement. "For every positive integer n, if n is prime, then 12 and $n^3 - n^2 + n$ have a common factor."

13. Prove or disprove the following statement. "For all integers b, c, and d, if x is a rational number such that $x^2 + bx + c = d$, then x is an integer." (Hints: Are all the quantifiers given explicitly? It is ok to use the quadratic formula.)

14. Prove that there is no largest prime number.

15. Prove that if $f(x)$, $g(x)$ and $h(x)$ are functions from R^+ to R^+ such that $f(x) = O(g(x))$ and $g(x) = O(h(x))$, then $f(x) = O(h(x))$.

Chapter 4

Induction, Recursion, and Recurrences

4.1 Mathematical Induction

Smallest Counter-Examples

In Section 3.3, we saw one way of proving statements about infinite universes: we considered a "generic" member of the universe and derived the desired statement about that generic member. When our universe is the universe of integers, or is in a one-to-one correspondence with the integers, there is a second technique we can use.

Recall our our proof of Euclid's Division Theorem (Theorem 2.12), which says that for each pair (m,n) of positive integers, there are nonnegative integers q and r such that $m = nq+r$ and $0 \le r < n$. For the purpose of a proof by contradiciton, we assumed that the statement was fales. Then we said the following. "Among all pairs (m,n) that make it false, choose the smallest m that makes it false. We cannot have $m < n$ because then the statement would be true with $q = 0$ and $r = m$, and we cannot have $m = n$ because then the statement is true with $q = 1$ and $r = 0$. This means $m - n$ is a positive number smaller than m. We assumed that m was the smallest value that made the theorem false, and so the theorem must be true for the pair $(m-n,n)$. Therefore, there must exist a q' and r' such that

$$m - n = q'n + r', \text{ with } 0 \le r' < n.$$

Thus $m = (q'+1)n+r'$. Now, by setting $q = q'+1$ and $r = r'$, we can satisfy the theorem for the pair (m,n), contradicting the assumption that the statement is false. Thus the only possibility is that the statement is true."

Focus on the sentences "This means $m-n$ is a positive number smaller than m. We assumed that m was the smallest value that made the theorem false, and so the theorem must be true for the pair $(m-n,n)$. Therefore, there must exist a q' and r' such that

$$m - n = q'n + r', \text{ with } 0 \le r' < n.$$

Thus $m = (q'+1)n + r'$." To analyze these sentences, let $p(m,n)$ denote the statement "there are nonnegative integers q and r with $0 \le r < n$ such that $m = nq + r$" The quoted sentences we focused on provide a proof that $p(m-n,n) \Rightarrow p(m,n)$. This implication is the crux of the proof. Let us give an analysis of the proof that shows the pivotal role of this impliction.

- We assumed a counter-example with a smallest m existed.
- Then using the fact that $p(m',n)$ had to be true for every m' smaller than m, we chose $m' = m-n$, and observed that $p(m',n)$ had to be true.
- Then we used the implication $p(m-n,n) \Rightarrow p(m,n)$ to conclude the truth of $p(m,n)$.
- But we had assumed that $p(m,n)$ was false, so this is the assumption we contradicted in the proof by contradiction.

Exercise 4.1-1 In Chapter 1 we learned Gauss's trick for showing that for all positive integers n,

$$1+2+3+4+...+n = \frac{n(n+1)}{2}\ . \tag{4.1}$$

Use the technique of asserting that if there is a counter-example, there is a smallest counter-example and deriving a contradiction to prove that the sum is $n(n+1)/2$. What implication did you have to prove in the process?

Exercise 4.1-2 For what values of $n \geq 0$ do you think $2^{n+1} \geq n^2+2$? Use the technique of asserting there is a smallest counter-example and deriving a contradiction to prove you are right. What implication did you have to prove in the process?

Exercise 4.1-3 For what values of $n \geq 0$ do you think $2^{n+1} \geq n^2+3$? Is it possible to use the technique of asserting there is a smallest counter-example and deriving a contradiction to prove you are right? If so, do so and describe the implication you had to prove in the process. If not, why not?

Exercise 4.1-4 Would it make sense to say that if there is a counter example there is a *largest* counter-example and try to base a proof on this? Why or why not?

In Exercise 4.1-1, suppose the formula for the sum is false. Then there must be a smallest n such that the formula does not hold for the sum of the first n positive integers. Thus for any positive integer i smaller than n,

$$1+2+\cdots+i = \frac{i(i+1)}{2}. \tag{4.2}$$

Because $1 = 1 \cdot 2/2$, Equation 4.1 holds when $n=1$, and therefore the smallest counterexample is not when $n=1$. So $n>1$, and $n-1$ is one of the positive integers i for which the formula holds. Substituting $n-1$ for i in Equation 4.2 gives us

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

Adding n to both sides gives

$$\begin{aligned} 1+2+\cdots+n-1+n &= \frac{(n-1)n}{2}+n \\ &= \frac{n^2-n+2n}{2} \\ &= \frac{n(n+1)}{2}\ . \end{aligned}$$

Thus n is not a counter-example after all, and therefore there is no counter-example to the formula. Thus the formula holds for all positive integers n. Note that the crucial step was proving that $p(n-1) \Rightarrow p(n)$, where $p(n)$ is the formula

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

In Exercise 4.1-2, let $p(n)$ be the statement that $2^{n+1} \geq n^2 + 2$. Some experimenting with small values of n leads us to believe this statement is true for all nonnegative integers. Thus we want to prove $p(n)$ is true for all nonnegative integers n. To do so, we assume that the statement that "$p(n)$ is true for all nonnegative integers n" is false. When a "for all" statement is false, there must be some n for which it is false. Therefore, there is some smallest nonnegative integer n so that $2^{n+1} \not\geq n^2 + 2$. Assume now that n has this value. This means that for all nonnegative integers i with $i < n$, $2^{i+1} \geq i^2 + 2$. Since we know from our experimentation that $n \neq 0$, we know $n - 1$ is a nonnegative integer less than n, so using $n - 1$ in place of i, we get

$$2^{(n-1)+1} \geq (n-1)^2 + 2,$$

or

$$\begin{aligned} 2^n &\geq n^2 - 2n + 1 + 2 \\ &= n^2 - 2n + 3. \end{aligned} \tag{4.3}$$

From this we want to draw a contradiction, presumably a contradiction to $2^{n+1} \not\geq n^2 + 2$.

To get the contradiction, we want to convert the left-hand side of Equation 4.3 to 2^{n+1}. For this purpose, we multiply both sides by 2, giving

$$\begin{aligned} 2^{n+1} &= 2 \cdot 2^n \\ &\geq 2n^2 - 4n + 6\ . \end{aligned}$$

You may have gotten this far and wondered "What next?" Since we want to obtain a contradiction, we want to convert the right hand side into something like $n^2 + 2$. More precisely, we will convert the right-hand side into $n^2 + 2$ plus an additional term. If we can show that the additional term is nonnegative, the proof will be complete. Thus we write

$$\begin{aligned} 2^{n+1} &\geq 2n^2 - 4n + 6 \\ &= (n^2 + 2) + (n^2 - 4n + 4) \\ &= n^2 + 2 + (n-2)^2 \\ &\geq n^2 + 2\ , \end{aligned} \tag{4.4}$$

since $(n-2)^2 \geq 0$. This is a contradiction, so there must not have been a smallest counter-example, and thus there must be no counter-example. Therefore $2^n \geq n^2 + 2$ for all nonnegative integers n.

What implication did we prove above? Let $p(n)$ stand for $2^{n+1} \geq n^2 + 2$. Then in Equations 4.3 and 4.4 we proved that $p(n-1) \Rightarrow p(n)$. Notice that at one point in our proof we had to note that we had considered the case with $n = 0$ already. Although we have given a proof by smallest counterexample, it is natural to ask whether it would make more sense to try to prove the statement directly. Would it make more sense to forget about the contradiction now that we have $p(n-1) \Rightarrow p(n)$ in hand and just observe that $p(0)$ and $p(n-1) \Rightarrow p(n)$ implies $p(1)$,that $p(1)$ and $p(n-1) \Rightarrow p(n)$ implies $p(2)$, and so on so that we have $p(k)$ for every k? We will address this question shortly.

Now let's consider Exercise 4.1-3. Notice that $2^{n+1} \not> n^2+3$ for $n = 0$ and 1, but $2^{n+1} > n^2+3$ for any larger n we look at at. Let us try to prove that $2^{n+1} > n^2 + 3$ for $n \geq 2$. We now let $p'(n)$ be the statement $2^{n+1} > n^2 + 3$. We can easily prove $p'(2)$: since $8 = 2^3 \geq 2^2 + 3 = 7$. Now suppose that among the integers larger than 2 there is a counter-example m to $p'(n)$. That is, suppose that there is an m such that $m > 2$ and $p'(m)$ is false. Then there is a smallest such m, so that for k between 2 and $m-1$, $p'(k)$ is true. If you look back at your proof that $p(n-1) \Rightarrow p(n)$, you will see that, when $n \geq 2$, essentially the same proof applies to p' as well. That is, with very similar computations we can show that $p'(n-1) \Rightarrow p'(n)$, so long as $n \geq 2$. Thus since $p'(m-1)$ is true, our implication tells us that $p'(m)$ is also true. This is a contradiction to our assumption that $p'(m)$ is false. therefore, $p'(m)$ is true. Again, we could conclude from $p'(2)$ and $p'(2) \Rightarrow p'(3)$ that $p'(3)$ is true, and similarly for $p'(4)$, and so on. The implication we had to prove was $p'(n-1) \Rightarrow p'(n)$.

For Exercise 4.1-4 if we have a counter-example to a statement $p(n)$ about an integer n, this means that there is an m such that $p(m)$ is false. To find a smallest counter example we would need to examine $p(0)$, $p(1)$, ..., perhaps all the way up to $p(m)$ in order to find a smallest counter-example, that is a smallest number k such that $p(k)$ is false. Since this involves only a finite number of cases, it makes sense to assert that there is a smallest counter-example. But, in answer to Exercise 4.1-4, it does not make sense to assert that there is a largest counter example, because there are infinitely many cases n that we would have to check in hopes if finding a largest one, and thus we might never find one. Even if we found one, we wouldn't be able to figure out that we had a largest counter-example just by checking larger and larger values of n, because we would never run out of values of n to check. Sometimes there is a largest counter-example, as in Exercise 4.1-3. To prove this, though, we didn't check all cases. Instead, based on our intuition, we guessed that the largest counter example was $n = 1$. Then we proved that we were right by showing that among numbers greater than or equal to two, there is no smallest counter-example. Sometimes there is no largest counter example n to a statement $p(n)$; for example $n^2 < n$ is false for all all integers n, and therefore there is no largest counter-example.

The Principle of Mathematical Induction

It may seem clear that repeatedly using the implication $p(n-1) \Rightarrow p(n)$ will prove $p(n)$ for all n (or all $n \geq 2$). That observation is the central idea of the Principle of Mathematical Induction, which we are about to introduce. In a theoretical discussion of how one constructs the integers from first principles, the principle of mathematical induction (or the equivalent principle that every set of nonnegative integers has a smallest element, thus letting us use the "smallest counter-example" technique) is one of the first principles we assume. The principle of mathematical induction is usually described in two forms. The one we have talked about so far is called the "weak form." It applies to statements about integers n.

The Weak Principle of Mathematical Induction. If the statement $p(b)$ is true, and the statement $p(n-1) \Rightarrow p(n)$ is true for all $n > b$, then $p(n)$ is true for all integers $n \geq b$.

Suppose, for example, we wish to give a direct inductive proof that $2^{n+1} > n^2 + 3$ for $n \geq 2$. We would proceed as follows. (The material in square brackets is not part of the proof; it is a running commentary on what is going on in the proof.)

> We shall prove by induction that $2^{n+1} > n^2 + 3$ for $n \geq 2$. First, $2^{2+1} = 2^3 = 8$, while $2^2 + 3 = 7$. [We just proved $p(2)$. We will now proceed to prove $p(n-1) \Rightarrow p(n)$.] Suppose now that $n > 2$ and that $2^n > (n-1)^2 + 3$. [We just made the hypothesis of $p(n-1)$ in order to use Rule 8 of our rules of inference.]
>
> Now multiply both sides of this inequality by 2, giving us
>
> $$\begin{aligned} 2^{n+1} &> 2(n^2 - 2n + 1) + 6 \\ &= n^2 + 3 + n^2 - 4n + 4 + 1 \\ &= n^2 + 3 + (n-2)^2 + 1\ . \end{aligned}$$
>
> Since $(n-2)^2 + 1$ is positive for $n > 2$, this proves $2^{n+1} > n^2 + 3$. [We just showed that from the hypothesis of $p(n-1)$ we can derive $p(n)$. Now we can apply Rule 8 to assert that $p(n-1) \Rightarrow p(n)$.] Therefore
>
> $$2^n > (n-1)^2 + 3 \quad \Rightarrow \quad 2^{n+1} > n^2 + 3.$$
>
> Therefore by the principle of mathematical induction, $2^{n+1} > n^2 + 3$ for $n \geq 2$.

In the proof we just gave, the sentence "First, $2^{2+1} = 2^3 = 8$, while $2^2 + 3 = 7$" is called the *base case*. It consisted of proving that $p(b)$ is true, where in this case b is 2 and $p(n)$ is $2^{n+1} > n^2 + 3$. The sentence "Suppose now that $n > 2$ and that $2^n > (n-1)^2 + 3$." is called the *inductive hypothesis*. This is the assumption that $p(n-1)$ is true. In inductive proofs, we always make such a hypothesis[1] in order to prove the implication $p(n-1) \Rightarrow p(n)$. The proof of the implication is called the *inductive step* of the proof. The final sentence of the proof is called the *inductive conclusion*.

Exercise 4.1-5 Use mathematical induction to show that

$$1 + 3 + 5 + \cdots + (2k-1) = k^2$$

for each positive integer k.

Exercise 4.1-6 For what values of n is $2^n > n^2$? Use mathematical induction to show that your answer is correct.

For Exercise 4.1-5, we note that the formula holds when $k = 1$. Assume inductively that the formula holds when $k = n - 1$, so that $1 + 3 + \cdots + (2n-3) = (n-1)^2$. Adding $2n - 1$ to both sides of this equation gives

$$\begin{aligned} 1 + 3 + \cdots + (2n-3) + (2n-1) &= n^2 - 2n + 1 + 2n - 1 \\ &= n^2. \end{aligned} \tag{4.5}$$

Thus the formula holds when $k = n$, and so by the principle of mathematical induction, the formula holds for all positive integers k.

[1] At times, it might be more convenient to assume that $p(n)$ is true and use this assumption to prove that $p(n+1)$ is true. This proves the implication $p(n) \Rightarrow p(n+1)$, which lets us reason in the same way.

Notice that in our discussion of Exercise 4.1-5 we nowhere mentioned a statement $p(n)$. In fact, $p(n)$ is the statement we get by substituting n for k in the formula, and in Equation 4.5 we were proving $p(n-1) \Rightarrow p(n)$. Next notice that we did not explicitly say we were going to give a proof by induction; instead we told the reader when we were making the inductive hypothesis by saying "Assume inductively that ...." This convention makes the prose flow nicely but still tells the reader that he or she is reading a proof by induction. Notice also how the notation in the statement of the exercise helped us write the proof. If we state what we are trying to prove in terms of a variable other than n, say k, then we can assume that our desired statement holds when this variable (k) is $n-1$ and then prove that the statement holds when $k = n$. Without this notational device, we have to either mention our statement $p(n)$ explicitly, or avoid any discussion of substituting values into the formula we are trying to prove. Our proof above that $2^{n+1} > n^2 + 3$ demonstrates this last approach to writing an inductive proof in plain English. This is usually the "slickest" way of writing an inductive proof, but it is often the hardest to master. We will use this approach first for the next exercise.

For Exercise 4.1-6 we note that $2 = 2^1 > 1^2 = 1$, but then the inequality fails for $n = 2, 3, 4$. However, $32 > 25$. Now we assume inductively that for $n > 5$ we have $2^{n-1} > (n-1)^2$. Multiplying by 2 gives us

$$\begin{aligned} 2^n > 2(n^2 - 2n + 1) &= n^2 + n^2 - 4n + 2 \\ &> n^2 + n^2 - n \cdot n \\ &= n^2 \ , \end{aligned}$$

since $n > 5$ implies that $-4n > -n \cdot n$. (We also used the fact that $n^2+n^2-4n+2 > n^2+n^2-4n$.) Thus by the principle of mathematical induction, $2^n > n^2$ for all $n \geq 5$.

Alternatively, we could write the following. Let $p(n)$ denote the inequality $2^n > n^2$. Then $p(5)$ is true because $32 > 25$. Assume that $n > 5$ and $p(n-1)$ is true. This gives us $2^{n-1} > (n-1)^2$. Multiplying by 2 gives

$$\begin{aligned} 2^n &> 2(n^2 - 2n + 1) \\ &= n^2 + n^2 - 4n + 2 \\ &> n^2 + n^2 - n \cdot n \\ &= n^2 \ , \end{aligned}$$

since $n > 5$ implies that $-4n > -n \cdot n$. Therefore $p(n-1) \Rightarrow p(n)$. Thus by the principle of mathematical induction, $2^n > n^2$ for all $n \geq 5$.

Notice how the "slick" method simply assumes that the reader knows we are doing a proof by induction from our "Assume inductively. . . ," and mentally supplies the appropriate $p(n)$ and observes that we have proved $p(n-1) \Rightarrow p(n)$ at the right moment.

Here is a slight variation of the technique of changing variables. To prove that $2^n > n^2$ when $n \geq 5$, we observe that the inequality holds when $n = 5$ since $32 > 25$. Assume inductively that the inequality holds when $n = k$, so that $2^k > k^2$. Now when $k \geq 5$, multiplying both sides of this inequality by 2 yields

$$\begin{aligned} 2^{k+1} > 2k^2 &= k^2 + k^2 \\ &\geq k^2 + 5k \\ &> k^2 + 2k + 1 \\ &= (k+1)^2 \ , \end{aligned}$$

since $k \geq 5$ implies that $k^2 \geq 5k$ and $5k = 2k+3k > 2k+1$. Thus by the principle of mathematical induction, $2^n > n^2$ for all $n \geq 5$.

This last variation of the proof illustrates two ideas. First, there is no need to save the name n for the variable we use in applying mathematical induction. We used k as our "inductive variable" in this case. Second, as suggested in a footnote earlier, there is no need to restrict ourselves to proving the implication $p(n-1) \Rightarrow p(n)$. In this case, we proved the implication $p(k) \Rightarrow p(k+1)$. Clearly these two implications are equivalent as n ranges over all integers larger than b and as k ranges over all integers larger than or equal to b.

Strong Induction

In our proof of Euclid's division theorem we had a statement of the form $p(m,n)$ and, assuming that it was false, we chose a smallest m such that $p(m,n)$ is false for some n. This meant we could assume that $p(m',n)$ is true for **all** $m' < m$, and we needed this assumption, because we ended up showing that $p(m-n,n) \Rightarrow p(m,n)$ in order to get our contradiction. This situation differs from the examples we used to introduce mathematical induction, for in those we used an implication of the form $p(n-1) \Rightarrow p(n)$. The essence of our method in proving Euclid's division theorem is that we have a statement $q(k)$ we want to prove. We suppose it is false, so that there must be a smallest k for which $q(k)$ is false. This means we may assume $q(k')$ is true for **all** k' in the universe of q with $k' < k$. We then use this assumption to derive a proof of $q(k)$, thus generating our contradiction.

Again, we can avoid the step of generating a contradiction in the following way. Suppose first we have a proof of $q(0)$. Suppose also that we have a proof that

$$q(0) \wedge q(1) \wedge q(2) \wedge \ldots \wedge q(k-1) \Rightarrow q(k)$$

for all k larger than 0. Then from $q(0)$ we can prove $q(1)$, from $q(0) \wedge q(1)$ we can prove $q(2)$, from $q(0) \wedge q(1) \wedge q(2)$ we can prove $q(3)$ and so on, giving us a proof of $q(n)$ for any n we desire. This is another form of the mathematical induction principle. We use it when, as in Euclid's division theorem, we can get an implication of the form $q(k') \Rightarrow q(k)$ for *some* $k' < k$ or when we can get an implication of the form $q(0) \wedge q(1) \wedge q(2) \wedge \ldots \wedge q(k-1) \Rightarrow q(k)$. (As is the case in Euclid's division theorem, we often don't really know what the k' is, so in these cases the first kind of situation is really just a special case of the second. Thus, we do not treat the first of the two implications separately.) We have described the method of proof known as the Strong Principle of Mathematical Induction.

The Strong Principle of Mathematical Induction. If the statement $p(b)$ is true, and the statement $p(b) \wedge p(b+1) \wedge \ldots \wedge p(n-1) \Rightarrow p(n)$ is true for all $n > b$, then $p(n)$ is true for all integers $n \geq b$.

Exercise 4.1-7 Prove that every positive integer is either a power of a prime number or the product of powers of prime numbers.

In Exercise 4.1-7 we can observe that 1 is a power of a prime number; for example $1 = 2^0$. Suppose now we know that every number less than n is a power of a prime number or a product of powers of prime numbers. Then if n is not a prime number, it is a product of two smaller numbers, each of which is, by our supposition, a power of a prime number or a product of powers of prime numbers. Therefore n is a power of a prime number or a product of powers of prime numbers. Thus, by the strong principle of mathematical induction, every positive integer is a power of a prime number or a product of powers of prime numbers.

Note that there was no explicit mention of an implication of the form

$$p(b) \wedge p(b+1) \wedge \ldots \wedge p(n-1) \Rightarrow p(n) .$$

This is common with inductive proofs. Note also that we did not explicitly identify the base case or the inductive hypothesis in our proof. This is common too. Readers of inductive proofs are expected to recognize when the base case is being given and when an implication of the form $p(n-1) \Rightarrow p(n)$ or $p(b) \wedge p(b+1) \wedge \cdots \wedge p(n-1) \Rightarrow p(n)$ is being proved.

Mathematical induction is used frequently in discrete math and computer science. Many quantities that we are interested in measuring, such as running time, space, or output of a program, typically are restricted to positive integers, and thus mathematical induction is a natural way to prove facts about these quantities. We will use it frequently throughout this book. We typically will not distinguish between strong and weak induction, we just think of them both as induction. (In Problems 14 and 15 at the end of the section you will be asked to derive each version of the principle from the other.)

Induction in general

To summarize what we have said so far, a typical proof by mathematical induction showing that a statement $p(n)$ is true for all integers $n \geq b$ consists of three steps.

1. First we show that $p(b)$ is true. This is called "establishing a *base case*."

2. Then we show either that for all $n > b$, $p(n-1) \Rightarrow p(n)$, or that for all $n > b$,

   $$p(b) \wedge p(b+1) \wedge \ldots \wedge p(n-1) \Rightarrow p(n).$$

   For this purpose, we make either the *inductive hypothesis* of $p(n-1)$ or the *inductive hypothesis* $p(b) \wedge p(b+1) \wedge \ldots \wedge p(n-1)$. Then we derive $p(n)$ to complete the proof of the implication we desire, either $p(n-1) \Rightarrow p(n)$ or $p(b) \wedge p(b+1) \wedge \ldots \wedge p(n-1) \Rightarrow p(n)$.

   Instead we could

2.′ show either that for all $n \geq b$, $p(n) \Rightarrow p(n+1)$ or

   $$p(b) \wedge p(b+1) \wedge \cdots \wedge p(n) \Rightarrow p(n+1).$$

   For this purpose, we make either the *inductive hypothesis* of $p(n)$ or the *inductive hypothesis* $p(b) \wedge p(b+1) \wedge \ldots \wedge p(n)$. Then we derive $p(n=1)$ to complete the proof of the implication we desire, either $p(n) \Rightarrow p(n=1)$ or $p(b) \wedge p(b+1) \wedge \ldots \wedge p(n) \Rightarrow p(n=1)$.

3. Finally, we conclude on the basis of the principle of mathematical induction that $p(n)$ is true for all integers n greater than or equal to b.

The second step is the core of an inductive proof. This is usually where we need the most insight into what we are trying to prove. In light of our discussion of Exercise 4.1-6, it should be clear that step $2'$ is simply a variation on the theme of writing an inductive proof.

It is important to realize that induction arises in some circumstances that do not fit the "pat" typical description we gave above. These circumstances seem to arise often in computer science. However, inductive proofs always involve three things. First we always need a base case or cases. Second, we need to show an implication that demonstrates that $p(n)$ is true given that $p(n')$ is true for some set of $n' < n$, or possibly we may need to show a set of such implications. Finally, we reach a conclusion on the basis of the first two steps.

For example, consider the problem of proving the following statement:

$$\sum_{i=0}^{n} \left\lfloor \frac{i}{2} \right\rfloor = \begin{cases} \frac{n^2}{4} & \text{if } n \text{ is even} \\ \frac{n^2-1}{4} & \text{if } n \text{ is odd} \end{cases} \tag{4.6}$$

In order to prove this, one must show that $p(0)$ is true, $p(1)$ is true, $p(n-2) \Rightarrow p(n)$ if n is odd, and that $p(n-2) \Rightarrow p(n)$, if n is even. Putting all these together, we see that our formulas hold for all $n \geq 0$. We can view this as either two proofs by induction, one for even and one for odd numbers, or one proof in which we have two base cases and two methods of deriving results from previous ones. This second view is more profitable, because it expands our view of what induction means, and makes it easier to find inductive proofs. In particular we could find situations where we have just one implication to prove but several base cases to check to cover all cases, or just one base case, but several different implications to prove to cover all cases.

Logically speaking, we could rework the example above so that it fits the pattern of strong induction. For example, when we prove a second base case, then we have just proved that the first base case implies it, because a true statement implies a true statement. Writing a description of mathematical induction that covers all kinds of base cases and implications one might want to consider in practice would simply give students one more unnecessary thing to memorize, so we shall not do so. However, in the mathematics literature and especially in the computer science literature, inductive proofs are written with multiple base cases and multiple implications with no effort to reduce them to one of the standard forms of mathematical induction. So long as it is possible to "cover" all the cases under consideration with such a proof, it can be rewritten as a standard inductive proof. Since readers of such proofs are expected to know this is possible, and since it adds unnecessary verbiage to a proof to do so, this is almost always left out.

Important Concepts, Formulas, and Theorems

1. *Weak Principle of Mathematical Induction.* The weak principle of mathematical induction states that

    If the statement $p(b)$ is true, and the statement $p(n-1) \Rightarrow p(n)$ is true for all $n > b$, then $p(n)$ is true for all integers $n \geq b$.

2. *Strong Principle of Mathematical Induction.* The strong principle of mathematical induction states that

    If the statement $p(b)$ is true, and the statement $p(b) \wedge p(b+1) \wedge \ldots \wedge p(n-1) \Rightarrow p(n)$ is true for all $n > b$, then $p(n)$ is true for all integers $n \geq b$.

3. *Base Case.* Every proof by mathematical induction, strong or weak, begins with a *base case* which establishes the result being proved for at least one value of the variable on which we are inducting. This base case should prove the result for the smallest value of the variable for which we are asserting the result. In a proof with multiple base cases, the base cases should cover all values of the variable which are not covered by the inductive step of the proof.

4. *Inductive Hypothesis.* Every proof by induction includes an inductive hypothesis in which we assume the result $p(n)$ we are trying to prove is true when $n = k - 1$ or when $n < k$ (or in which we assume an equivalent statement).

5. *Inductive Step.* Every proof by induction includes an inductive step in which we prove the implication that $p(k-1) \Rightarrow p(k)$ or the implication that $p(b) \wedge p(b+1) \wedge \cdots \wedge p(k-1) \Rightarrow p(k)$, or some equivalent implication.

6. *Inductive Conclusion.* A proof by mathematical induction should include, at least implicitly, a concluding statement of the form "Thus by the principle of mathematical induction ...," which asserts that by the principle of mathematical induction the result $p(n)$ which we are trying to prove is true for all values of n including and beyond the base case(s).

Problems

1. This exercise explores ways to prove that $\frac{2}{3} + \frac{2}{9} + \cdots + \frac{2}{3^n} = 1 - \left(\frac{1}{3}\right)^n$ for all positive integers n.

   (a) First, try proving the formula by contradiction. Thus you assume that there is some integer n that makes the formula false. Then there must be some smallest n that makes the formula false. Can this smallest n be 1? What do we know about $\frac{2}{3} + \frac{2}{9} + \cdots + \frac{2}{3^i}$ when i is a positive integer smaller than this smallest n? Is $n - 1$ a positive integer for this smallest n? What do we know about $\frac{2}{3} + \frac{2}{9} + \cdots + \frac{2}{3^{n-1}}$ for this smallest n? Write this as an equation and add $\frac{2}{3^n}$ to both sides and simplify the right side. What does this say about our assumption that the formula is false? What can you conclude about the truth of the formula? If $p(k)$ is the statement $\frac{2}{3} + \frac{2}{9} + \cdots + \frac{2}{3^k} = 1 - \left(\frac{1}{3}\right)^k$, what implication did we prove in the process of deriving our contradiction?

   (b) What is the base step in a proof by mathematical induction that $\frac{2}{3} + \frac{2}{9} + \cdots + \frac{2}{3^n} = 1 - \left(\frac{1}{3}\right)^n$ for all positive integers n? What would you assume as an inductive hypothesis? What would you prove in the inductive step of a proof of this formula by induction? Prove it. What does the principle of mathematical induction allow you to conclude? If $p(k)$ is the statement $\frac{2}{3} + \frac{2}{9} + \cdots + \frac{2}{3^k} = 1 - \left(\frac{1}{3}\right)^k$, what implication did we prove in the process of doing our proof by induction?

2. Use contradiction to prove that $1 \cdot 2 + 2 \cdot 3 + \cdots + n(n+1) = \frac{n(n+1)(n+2)}{3}$.

3. Use induction to prove that $1 \cdot 2 + 2 \cdot 3 + \cdots + n(n+1) = \frac{n(n+1)(n+2)}{3}$.

4. Prove that $1^3 + 2^3 + 3^3 + \cdots + n^3 = \frac{n^2(n+1)^2}{4}$.

5. Write a careful proof of Euclid's division theorem using strong induction.

6. Prove that $\sum_{i=j}^{n}\binom{i}{j} = \binom{n+1}{j+1}$. As well as the inductive proof that we are expecting, there is a nice "story" proof of this formula. It is well worth trying to figure it out.

7. Prove that every number greater than 7 is a sum of a nonnegative integer multiple of 3 and a nonnegative integer multiple of 5.

8. The usual definition of exponents in an advanced mathematics course (or an intermediate computer science course) is that $a^0 = 1$ and $a^{n+1} = a^n \cdot a$. Explain why this defines a^n for all nonnegative integers n. Prove the rule of exponents $a^{m+n} = a^m a^n$ from this definition.

9. Our arguments in favor of the sum principle were quite intuitive. In fact the sum principle for n sets follows from the sum principle for two sets. Use induction to prove the sum principle for a union of n sets from the sum principle for a union of two sets.

10. We have proved that every positive integer is a power of a prime number or a product of powers of prime numbers. Show that this factorization is unique in the following sense: If you have two factorizations of a positive integer, both factorizations use exactly the same primes, and each prime occurs to the same power in both factorizations. For this purpose, it is helpful to know that if a prime divides a product of integers, then it divides one of the integers in the product. (Another way to say this is that if a prime is a factor of a product of integers, then it is a factor of one of the integers in the product.)

11. Prove that $1^4 + 2^4 + \cdots + n^4 = O(n^5 - n^4)$.

12. Find the error in the following "proof" that all positive integers n are equal. Let $p(n)$ be the statement that all numbers in an n-element set of positive integers are equal. Then $p(1)$ is true. Now assume $p(n-1)$ is true, and let N be the set of the first n integers. Let N' be the set of the first $n-1$ integers, and let N'' be the set of the last $n-1$ integers. Then by $p(n-1)$ all members of N' are equal and all members of N'' are equal. Thus the first $n-1$ elements of N are equal and the last $n-1$ elements of N are equal, and so all elements of N are equal. Thus all positive integers are equal.

13. Prove by induction that the number of subsets of an n-element set is 2^n.

14. Prove that the Strong Principle of Mathematical Induction implies the Weak Principle of Mathematical Induction.

15. Prove that the Weak Principal of Mathematical Induction implies the Strong Principal of Mathematical Induction.

16. Prove (4.6).

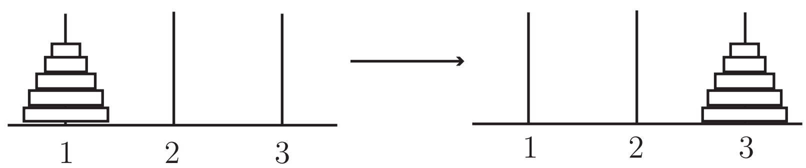
4.2 Recursion, Recurrences and Induction

Recursion

Exercise 4.2-1 Describe the uses you have made of recursion in writing programs. Include as many as you can.

Exercise 4.2-2 Recall that in the Towers of Hanoi problem we have three pegs numbered 1, 2 and 3, and on one peg we have a stack of n disks, each smaller in diameter than the one below it as in Figure 4.1. An allowable move consists of removing a disk

Figure 4.1: The Towers of Hanoi



from one peg and sliding it onto another peg so that it is not above another disk of smaller size. We are to determine how many allowable moves are needed to move the disks from one peg to another. Describe the strategy you have used or would use in a recursive program to solve this problem.

For the Tower of Hanoi problem, to solve the problem with no disks you do nothing. To solve the problem of moving all disks to peg 2, we do the following

1. (Recursively) solve the problem of moving $n-1$ disks from peg 1 to peg 3,
2. move disk n to peg 2,
3. (Recursively) solve the problem of moving $n-1$ disks on peg 3 to peg 2.

Thus if $M(n)$ is the number of moves needed to move n disks from peg i to peg j, we have

$$M(n) = 2M(n-1) + 1.$$

This is an example of a **recurrence equation** or **recurrence**. A recurrence equation for a function defined on the set of integers greater than or equal to some number b is one that tells us how to compute the nth value of a function from the $(n-1)$st value or some or all the values preceding n. To completely specify a function on the basis of a recurrence, we have to give enough information about the function to get started. This information is called the *initial condition (or the initial conditions)* (which we also call the *base case*) for the recurrence. In this case we have said that $M(0) = 0$. Using this, we get from the recurrence that $M(1) = 1$, $M(2) = 3$, $M(3) = 7$, $M(4) = 15$, $M(5) = 31$, and are led to guess that $M(n) = 2^n - 1$.

Formally, we write our recurrence and initial condition together as

$$M(n) = \begin{cases} 0 & \text{if } n = 0 \\ 2M(n-1) + 1 & \text{otherwise} \end{cases} \tag{4.7}$$

Now we give an inductive proof that our guess is correct. The base case is trivial, as we have defined $M(0) = 0$, and $0 = 2^0 - 1$. For the inductive step, we assume that $n > 0$ and $M(n-1) = 2^{n-1} - 1$. From the recurrence, $M(n) = 2M(n-1) + 1$. But, by the inductive hypothesis, $M(n-1) = 2^{n-1} - 1$, so we get that:

$$\begin{aligned} M(n) &= 2M(n-1) + 1 && (4.8) \\ &= 2(2^{n-1} - 1) + 1 && (4.9) \\ &= 2^n - 1. && (4.10) \end{aligned}$$

thus by the principle of mathematical induction, $M(n) = 2^n - 1$ for all nonnegative integers n.

The ease with which we solved this recurrence and proved our solution correct is no accident. Recursion, recurrences and induction are all intimately related. The relationship between recursion and recurrences is reasonably transparent, as recurrences give a natural way of analyzing recursive algorithms. Recursion and recurrences are abstractions that allow you to specify the solution to an instance of a problem of size n as some function of solutions to smaller instances. Induction also falls naturally into this paradigm. Here, you are deriving a statement $p(n)$ from statements $p(n')$ for $n' < n$. Thus we really have three variations on the same theme.

We also observe, more concretely, that the mathematical correctness of solutions to recurrences is naturally proved via induction. In fact, the correctness of recurrences in describing the number of steps needed to solve a recursive problem is also naturally proved by induction. The recurrence or recursive structure of the problem makes it straightforward to set up the induction proof.

First order linear recurrences

Exercise 4.2-3 The empty set ($\emptyset$) is a set with no elements. How many subsets does it have? How many subsets does the one-element set $\{1\}$ have? How many subsets does the two-element $\{1, 2\}$ set have? How many of these contain 2? How many subsets does $\{1, 2, 3\}$ have? How many contain 3? Give a recurrence for the number $S(n)$ of subsets of an n-element set, and prove by induction that your recurrence is correct.

Exercise 4.2-4 When someone is paying off a loan with initial amount A and monthly payment M at an interest rate of p percent, the total amount $T(n)$ of the loan after n months is computed by adding $p/12$ percent to the amount due after $n-1$ months and then subtracting the monthly payment M. Convert this description into a recurrence for the amount owed after n months.

Exercise 4.2-5 Given the recurrence

$$T(n) = rT(n-1) + a,$$

where r and a are constants, find a recurrence that expresses $T(n)$ in terms of $T(n-2)$ instead of $T(n-1)$. Now find a recurrence that expresses $T(n)$ in terms of $T(n-3)$ instead of $T(n-2)$ or $T(n-1)$. Now find a recurrence that expresses $T(n)$ in terms of $T(n-4)$ rather than $T(n-1)$, $T(n-2)$, or $T(n-3)$. Based on your work so far, find a general formula for the solution to the recurrence

$$T(n) = rT(n-1) + a,$$

with $T(0) = b$, and where r and a are constants.

If we construct small examples for Exercise 4.2-3, we see that $\emptyset$ has only 1 subset, $\{1\}$ has 2 subsets, $\{1,2\}$ has 4 subsets, and $\{1,2,3\}$ has 8 subsets. This gives us a good guess as to what the general formula is, but in order to prove it we will need to think recursively. Consider the subsets of $\{1,2,3\}$:

$$\begin{array}{cccc} \emptyset & \{1\} & \{2\} & \{1,2\} \\ \{3\} & \{1,3\} & \{2,3\} & \{1,2,3\} \end{array}$$

The first four subsets do not contain three, and the second four do. Further, the first four subsets are exactly the subsets of $\{1,2\}$, while the second four are the four subsets of $\{1,2\}$ with 3 added into each one. This suggests that the recurrence for the number of subsets of an n-element set (which we may assume is $\{1,2,\ldots,n\}$) is

$$S(n) = \begin{cases} 2S(n-1) & \text{if } n \geq 1 \\ 1 & \text{if } n = 0 \end{cases}. \tag{4.11}$$

To prove this recurrence is correct, we note that the subsets of an n-element set can be partitioned by whether they contain element n or not. The subsets of $\{1,2,\ldots,n\}$ containing element n can be constructed by adjoining the element n to the subsets not containing element n. So the number of subsets containing element n is the same as the number of subsets not containing element n. The number of subsets not containing element n is just the number of subsets of an $n-1$-element set. Therefore each block of our partition has size equal to the number of subsets of an $n-1$-element set. Thus, by the sum principle, the number of subsets of $\{1,2,\ldots,n\}$ is twice the number of subsets of $\{1,2,\ldots,n-1\}$. This proves that $S(n) = 2S(n-1)$ if $n > 0$. We already observed that $\emptyset$ has no subsets, so we have proved the correctness of Recurrence 4.11.

For Exercise 4.2-4 we can algebraically describe what the problem said in words by

$$T(n) = (1 + .01p/12) \cdot T(n-1) - M,$$

with $T(0) = A$. Note that we add $.01p/12$ times the principal to the amount due each month, because $p/12$ percent of a number is $.01p/12$ times the number.

Iterating a recurrence

Turning to Exercise 4.2-5, we can substitute the right hand side of the equation $T(n-1) = rT(n-2) + a$ for $T(n-1)$ in our recurrence, and then substitute the similar equations for $T(n-2)$ and $T(n-3)$ to write

$$\begin{aligned} T(n) &= r(rT(n-2)+a)+a \\ &= r^2T(n-2)+ra+a \\ &= r^2(rT(n-3)+a)+ra+a \\ &= r^3T(n-3)+r^2a+ra+a \\ &= r^3(rT(n-4)+a)+r^2a+ra+a \\ &= r^4T(n-4)+r^3a+r^2a+ra+a \end{aligned}$$

From this, we can guess that

$$\begin{aligned} T(n) &= r^n T(0) + a\sum_{i=0}^{n-1} r^i \\ &= r^n b + a\sum_{i=0}^{n-1} r^i. \end{aligned} \tag{4.12}$$

The method we used to guess the solution is called *iterating the recurrence* because we repeatedly use the recurrence with smaller and smaller values in place of n. We could instead have written

$$\begin{aligned} T(0) &= b \\ T(1) &= rT(0) + a \\ &= rb + a \\ T(2) &= rT(1) + a \\ &= r(rb + a) + a \\ &= r^2 b + ra + a \\ T(3) &= rT(2) + a \\ &= r^3 b + r^2 a + ra + a \end{aligned}$$

This leads us to the same guess, so why have we introduced two methods? Having different approaches to solving a problem often yields insights we would not get with just one approach. For example, when we study recursion trees, we will see how to visualize the process of iterating certain kinds of recurrences in order to simplify the algebra involved in solving them.

Geometric series

You may recognize that sum $\sum_{i=0}^{n-1} r^i$ in Equation 4.12. It is called a *finite geometric series with common ratio* r. The sum $\sum_{i=0}^{n-1} ar^i$ is called a *finite geometric series with common ratio* r *and initial value* a. Recall from algebra the factorizations

$$\begin{aligned} (1-x)(1+x) &= 1-x^2 \\ (1-x)(1+x+x^2) &= 1-x^3 \\ (1-x)(1+x+x^2+x^3) &= 1-x^4 \end{aligned}$$

These factorizations are easy to verify, and they suggest that $(1-r)(1+r+r^2+\cdots+r^{n-1}) = 1-r^n$, or

$$\sum_{i=0}^{n-1} r^i = \frac{1-r^n}{1-r}. \tag{4.13}$$

In fact this formula is true, and lets us rewrite the formula we got for $T(n)$ in a very nice form.

Theorem 4.1 *If $T(n) = rT(n-1) + a$, $T(0) = b$, and $r \neq 1$ then*

$$T(n) = r^n b + a\frac{1-r^n}{1-r} \tag{4.14}$$

for all nonnegative integers n.

Proof: We will prove our formula by induction. Notice that the formula gives $T(0) = r^0 b + a\frac{1-r^0}{1-r}$ which is b, so the formula is true when $n = 0$. Now assume that $n > 0$ and

$$T(n-1) = r^{n-1}b + a\frac{1-r^{n-1}}{1-r}.$$

Then we have

$$\begin{aligned} T(n) &= rT(n-1) + a \\ &= r\left(r^{n-1}b + a\frac{1-r^{n-1}}{1-r}\right) + a \\ &= r^n b + \frac{ar - ar^n}{1-r} + a \\ &= r^n b + \frac{ar - ar^n + a - ar}{1-r} \\ &= r^n b + a\frac{1-r^n}{1-r}\ . \end{aligned}$$

Therefore by the principle of mathematical induction, our formula holds for all integers n greater than 0. ■

We did not prove Equation 4.13. However it is easy to use Theorem 4.1 to prove it.

Corollary 4.2 *The formula for the sum of a geometric series with $r \neq 1$ is*

$$\sum_{i=0}^{n-1} r^i = \frac{1-r^n}{1-r}. \tag{4.15}$$

Proof: Define $T(n) = \sum_{i=0}^{n-1} r^i$. Then $T(n) = rT(n-1) + 1$, and since $T(0)$ is a sum with no terms, $T(0) = 0$. Applying Theorem 4.1 with $b = 0$ and $a = 1$ gives us $T(n) = \frac{1-r^n}{1-r}$. ■

Often, when we see a geometric series, we will only be concerned with expressing the sum in big-O notation. In this case, we can show that the sum of a geometric series is at most the largest term times a constant factor, where the constant factor depends on r, but not on n.

Lemma 4.3 *Let r be a quantity whose value is independent of n and not equal to 1. Let $t(n)$ be the largest term of the geometric series*

$$\sum_{i=0}^{n-1} r^i.$$

Then the value of the geometric series is $O(t(n))$.

Proof: It is straightforward to see that we may limit ourselves to proving the lemma for $r > 0$. We consider two cases, depending on whether $r > 1$ or $r < 1$. If $r > 1$, then

$$\begin{aligned} \sum_{i=0}^{n-1} r^i &= \frac{r^n - 1}{r-1} \\ &\leq \frac{r^n}{r-1} \\ &= r^{n-1}\frac{r}{r-1} \\ &= O(r^{n-1}). \end{aligned}$$

On the other hand, if $r < 1$, then the largest term is $r^0 = 1$, and the sum has value

$$\frac{1-r^n}{1-r} < \frac{1}{1-r}.$$

Thus the sum is $O(1)$, and since $t(n) = 1$, the sum is $O(t(n))$. ■

In fact, when r is nonnegative, an even stronger statement is true. Recall that we said that, for two functions f and g from the real numbers to the real numbers that $f = \Theta(g)$ if $f = O(g)$ and $g = O(f)$.

Theorem 4.4 *Let r be a nonnegative quantity whose value is independent of n and not equal to 1. Let $t(n)$ be the largest term of the geometric series*

$$\sum_{i=0}^{n-1} r^i.$$

Then the value of the geometric series is $\Theta(t(n))$.

Proof: By Lemma 4.3, we need only show that $t(n) = O(\frac{r^n-1}{r-1})$. Since all r^i are nonnegative, the sum $\sum_{i=0}^{n-1} r^i$ is at least as large as any of its summands. But $t(n)$ is one of these summands, so $t(n) = O(\frac{r^n-1}{r-1})$. ■

Note from the proof that $t(n)$ and the constant in the big-O upper bound depend on r. We will use this Theorem in subsequent sections.

First order linear recurrences

A recurrence of the form $T(n) = f(n)T(n-1) + g(n)$ is called a *first order linear recurrence*. When $f(n)$ is a constant, say r, the general solution is almost as easy to write down as in the case we already figured out. Iterating the recurrence gives us

$$\begin{aligned}
T(n) &= rT(n-1) + g(n) \\
&= r\Big(rT(n-2) + g(n-1)\Big) + g(n) \\
&= r^2T(n-2) + rg(n-1) + g(n) \\
&= r^2\Big(rT(n-3) + g(n-2)\Big) + rg(n-1) + g(n) \\
&= r^3T(n-3) + r^2g(n-2) + rg(n-1) + g(n) \\
&= r^3\Big(rT(n-4) + g(n-3)\Big) + r^2g(n-2) + rg(n-1) + g(n) \\
&= r^4T(n-4) + r^3g(n-3) + r^2g(n-2) + rg(n-1) + g(n) \\
&\vdots \\
&= r^nT(0) + \sum_{i=0}^{n-1} r^i g(n-i)
\end{aligned}$$

This suggests our next theorem.

Theorem 4.5 *For any positive constants a and r, and any function g defined on the nonnegative integers, the solution to the first order linear recurrence*

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

is

$$T(n) = r^n a + \sum_{i=1}^{n} r^{n-i} g(i). \tag{4.16}$$

Proof: Let's prove this by induction.

Since the sum $\sum_{i=1}^{n} r^{n-i} g(i)$ in Equation 4.16 has no terms when $n = 0$, the formula gives $T(0) = 0$ and so is valid when $n = 0$. We now assume that n is positive and $T(n-1) = r^{n-1}a + \sum_{i=1}^{n-1} r^{(n-1)-i} g(i)$. Using the definition of the recurrence and the inductive hypothesis we get that

$$\begin{aligned} T(n) &= rT(n-1) + g(n) \\ &= r\left(r^{n-1}a + \sum_{i=1}^{n-1} r^{(n-1)-i} g(i)\right) + g(n) \\ &= r^n a + \sum_{i=1}^{n-1} r^{(n-1)+1-i} g(i) + g(n) \\ &= r^n a + \sum_{i=1}^{n-1} r^{n-i} g(i) + g(n) \\ &= r^n a + \sum_{i=1}^{n} r^{n-i} g(i). \end{aligned}$$

Therefore by the principle of mathematical induction, the solution to

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

is given by Equation 4.16 for all nonnegative integers n. ■

The formula in Theorem 4.5 is a little less easy to use than that in Theorem 4.1 because it gives us a sum to compute. Fortunately, for a number of commonly occurring functions g the sum $\sum_{i=1}^{n} r^{n-i} g(i)$ is reasonable to compute.

Exercise 4.2-6 Solve the recurrence $T(n) = 4T(n-1) + 2^n$ with $T(0) = 6$.

Exercise 4.2-7 Solve the recurrence $T(n) = 3T(n-1) + n$ with $T(0) = 10$.

For Exercise 4.2-6, using Equation 4.16, we can write

$$\begin{aligned} T(n) &= 6 \cdot 4^n + \sum_{i=1}^{n} 4^{n-i} \cdot 2^i \\ &= 6 \cdot 4^n + 4^n \sum_{i=1}^{n} 4^{-i} \cdot 2^i \end{aligned}$$

$$
\begin{aligned}
&= 6 \cdot 4^n + 4^n \sum_{i=1}^{n} \left(\frac{1}{2}\right)^i \\
&= 6 \cdot 4^n + 4^n \cdot \frac{1}{2} \cdot \sum_{i=0}^{n-1} \left(\frac{1}{2}\right)^i \\
&= 6 \cdot 4^n + (1 - (\frac{1}{2})^n) \cdot 4^n \\
&= 7 \cdot 4^n - 2^n
\end{aligned}
$$

For Exercise 4.2-7 we begin in the same way and face a bit of a surprise. Using Equation 4.16, we write

$$
\begin{aligned}
T(n) &= 10 \cdot 3^n + \sum_{i=1}^{n} 3^{n-i} \cdot i \\
&= 10 \cdot 3^n + 3^n \sum_{i=1}^{n} i3^{-i} \\
&= 10 \cdot 3^n + 3^n \sum_{i=1}^{n} i \left(\frac{1}{3}\right)^i . \qquad (4.17)
\end{aligned}
$$

Now we are faced with a sum that you may not recognize, a sum that has the form

$$\sum_{i=1}^{n} ix^i = x \sum_{i=1}^{n} ix^{i-1},$$

with $x = 1/3$. However by writing it in in this form, we can use calculus to recognize it as x times a derivative. In particular, using the fact that $0x^0 = 0$, we can write

$$\sum_{i=1}^{n} ix^i = x \sum_{i=0}^{n} ix^{i-1} = x \frac{d}{dx} \sum_{i=0}^{n} x^i = x \frac{d}{dx} \left(\frac{1 - x^{n+1}}{1 - x} \right).$$

But using the formula for the derivative of a quotient from calculus, we may write

$$x \frac{d}{dx} \left(\frac{1 - x^{n+1}}{1 - x} \right) = x \frac{(1-x)(-(n+1)x^n) - (1 - x^{n+1})(-1)}{(1-x)^2} = \frac{nx^{n+2} - (n+1)x^{n+1} + x}{(1-x)^2}.$$

Connecting our first and last equations, we get

$$\sum_{i=1}^{n} ix^i = \frac{nx^{n+2} - (n+1)x^{n+1} + x}{(1-x)^2}. \qquad (4.18)$$

Substituting in $x = 1/3$ and simplifying gives us

$$\sum_{i=1}^{n} i \left(\frac{1}{3}\right)^i = -\frac{3}{2}(n+1)\left(\frac{1}{3}\right)^{n+1} - \frac{3}{4}\left(\frac{1}{3}\right)^{n+1} + \frac{3}{4}.$$

Substituting this into Equation 4.17 gives us

$$
\begin{aligned}
T(n) &= 10 \cdot 3^n + 3^n \left(-\frac{3}{2}(n+1)\left(\frac{1}{3}\right)^{n+1} - \frac{3}{4}(1/3)^{n+1} + \frac{3}{4} \right) \\
&= 10 \cdot 3^n - \frac{n+1}{2} - \frac{1}{4} + \frac{3^{n+1}}{4} \\
&= \frac{43}{4} 3^n - \frac{n+1}{2} - \frac{1}{4}.
\end{aligned}
$$

The sum that arises in this exercise occurs so often that we give its formula as a theorem.

Theorem 4.6 *For any real number $x \neq 1$,*

$$\sum_{i=1}^{n} ix^i = \frac{nx^{n+2} - (n+1)x^{n+1} + x}{(1-x)^2}. \tag{4.19}$$

Proof: Given before the statement of the theorem.■

Important Concepts, Formulas, and Theorems

1. *Recurrence Equation or Recurrence.* A recurrence equation is one that tells us how to compute the nth term of a sequence from the $(n-1)$st term or some or all the preceding terms.

2. *Initial Condition.* To completely specify a function on the basis of a recurrence, we have to give enough information about the function to get started. This information is called the *initial condition (or the initial conditions)* for the recurrence.

3. *First Order Linear Recurrence.* A recurrence $T(n) = f(n)T(n-1) + g(n)$ is called a *first order linear recurrence.*

4. *Constant Coefficient Recurrence.* A recurrence in which $T(n)$ is expressed in terms of a sum of constant multiples of $T(k)$ for certain values $k < n$ (and perhaps another function of n) is called a *constant coefficient recurrence.*

5. *Solution to a First Order Constant Coefficient Linear Recurrence.* If $T(n) = rT(n-1) + a$, $T(0) = b$, and $r \neq 1$ then
$$T(n) = r^n b + a\frac{1-r^n}{1-r}$$
for all nonnegative integers n.

6. *Finite Geometric Series.* A finite geometric series with common ratio r is a sum of the form $\sum_{i=0}^{n-1} r^i$. The formula for the sum of a geometric series with $r \neq 1$ is
$$\sum_{i=0}^{n-1} r^i = \frac{1-r^n}{1-r}.$$

7. *Big-Theta Bounds on the Sum of a Geometric Series.* Let r be a nonnegative quantity whose value is independent of n and not equal to 1. Let $t(n)$ be the largest term of the geometric series
$$\sum_{i=0}^{n-1} r^i.$$
Then the value of the geometric series is $\Theta(t(n))$.

8. *Solution to a First Order Linear Recurrence.* For any positive constants a and r, and any function g defined on the nonnegative integers, the solution to the first order linear recurrence
$$T(n) = \begin{cases} rT(n-1) + g(n) & \text{if } n > 0 \\ a & \text{if } n = 0 \end{cases}$$
is
$$T(n) = r^n a + \sum_{i=1}^{n} r^{n-i} g(i).$$

9. *Iterating a Recurrence.* We say we are *iterating* a recurrence when we guess its solution by using the equation that expresses $T(n)$ in terms of $T(k)$ for k smaller than n to re-express $T(n)$ in terms of $T(k)$ for k smaller than $n-1$, then for k smaller than $n-2$, and so on until we can guess the formula for the sum.

10. *An Important Sum.* For any real number $x \neq 1$,
$$\sum_{i=1}^{n} ix^i = \frac{nx^{n+2} - (n+1)x^{n+1} + x}{(1-x)^2}.$$

Problems

1. Prove Equation 4.15 directly by induction.

2. Prove Equation 4.18 directly by induction.

3. Solve the recurrence $M(n) = 2M(n-1) + 2$, with a base case of $M(1) = 1$. How does it differ from the solution to Recurrence 4.7?

4. Solve the recurrence $M(n) = 3M(n-1) + 1$, with a base case of $M(1) = 1$. How does it differ from the solution to Recurrence 4.7.

5. Solve the recurrence $M(n) = M(n-1) + 2$, with a base case of $M(1) = 1$. How does it differ from the solution to Recurrence 4.7.

6. There are m functions from a one-element set to the set $\{1, 2, \ldots, m\}$. How many functions are there from a two-element set to $\{1, 2, \ldots, m\}$? From a three-element set? Give a recurrence for the number $T(n)$ of functions from an n-element set to $\{1, 2, \ldots, m\}$. Solve the recurrence.

7. Solve the recurrence that you derived in Exercise 4.2-4.

8. At the end of each year, a state fish hatchery puts 2000 fish into a lake. The number of fish in the lake at the beginning of the year doubles due to reproduction by the end of the year. Give a recurrence for the number of fish in the lake after n years and solve the recurrence.

9. Consider the recurrence $T(n) = 3T(n-1) + 1$ with the initial condition that $T(0) = 2$. We know that we could write the solution down from Theorem 4.1. Instead of using the theorem, try to guess the solution from the first four values of $T(n)$ and then try to guess the solution by iterating the recurrence four times.

10. What sort of big-Θ bound can we give on the value of a geometric series $1+r+r^2+\cdots+r^n$ with common ratio $r=1$?

11. Solve the recurrence $T(n) = 2T(n-1) + n2^n$ with the initial condition that $T(0) = 1$.

12. Solve the recurrence $T(n) = 2T(n-1) + n^3 2^n$ with the initial condition that $T(0) = 2$.

13. Solve the recurrence $T(n) = 2T(n-1) + 3^n$ with $T(0) = 1$.

14. Solve the recurrence $T(n) = rT(n-1) + r^n$ with $T(0) = 1$.

15. Solve the recurrence $T(n) = rT(n-1) + r^{2n}$ with $T(0) = 1$

16. Solve the recurrence $T(n) = rT(n-1) + s^n$ with $T(0) = 1$.

17. Solve the recurrence $T(n) = rT(n-1) + n$ with $T(0) = 1$.

18. The Fibonacci numbers are defined by the recurrence

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

   (a) Write down the first ten Fibonacci numbers.

   (b) Show that $(\frac{1+\sqrt{5}}{2})^n$ and $(\frac{1-\sqrt{5}}{2})^n$ are solutions to the equation $F(n) = F(n-1) + F(n-2)$.

   (c) Why is

$$c_1(\frac{1+\sqrt{5}}{2})^n + c_2(\frac{1-\sqrt{5}}{2})^n$$

   a solution to the equation $F(n) = F(n-1) + F(n-2)$ for any real numbers c_1 and c_2?

   (d) Find constants c_1 and c_2 such that the Fibonacci numbers are given by

$$F(n) = c_1(\frac{1+\sqrt{5}}{2})^n + c_2(\frac{1-\sqrt{5}}{2})^n$$

4.3 Growth Rates of Solutions to Recurrences

Divide and Conquer Algorithms

One of the most basic and powerful algorithmic techniques is *divide and conquer*. Consider, for example, the binary search algorithm, which we will describe in the context of guessing a number between 1 and 100. Suppose someone picks a number between 1 and 100, and allows you to ask questions of the form "Is the number greater than k?" where k is an integer you choose. Your goal is to ask as few questions as possible to figure out the number. Your first question should be "Is the number greater than 50?" Why is this? Well, after asking if the number is bigger than 50, you have learned either that the number is between one and 50, or that the number is between 51 and 100. In either case have reduced your problem to one in which the range is only half as big. Thus you have *divided* the problem up into a problem that is only half as big, and you can now (recursively) *conquer* this remaining problem. (If you ask any other question, the size of one of the possible ranges of values you could end up with would be more than half the size of the original problem.) If you continue in this fashion, always cutting the problem size in half, you will reduce the problem size down to one fairly quickly, and then you will know what the number is. Of course it would be easier to cut the problem size exactly in half each time if we started with a number in the range from one to 128, but the question doesn't sound quite so plausible then. Thus to analyze the problem we will assume someone asks you to figure out a number between 0 and n, where n is a power of 2.

Exercise 4.3-1 Let $T(n)$ be number of questions in binary search on the range of numbers between 1 and n. Assuming that n is a power of 2, give a recurrence for $T(n)$.

For Exercise 4.3-1 we get:

$$T(n) = \begin{cases} T(n/2) + 1 & \text{if } n \geq 2 \\ 1 & \text{if } n = 1 \end{cases} \tag{4.20}$$

That is, the number of guesses to carry out binary search on n items is equal to 1 step (the guess) plus the time to solve binary search on the remaining $n/2$ items.

What we are really interested in is how much time it takes to use binary search in a computer program that looks for an item in an ordered list. While the number of questions gives us a feel for the amount of time, processing each question may take several steps in our computer program. The exact amount of time these steps take might depend on some factors we have little control over, such as where portions of the list are stored. Also, we may have to deal with lists whose length is not a power of two. Thus a more realistic description of the time needed would be

$$T(n) \leq \begin{cases} T(\lceil n/2 \rceil) + C_1 & \text{if } n \geq 2 \\ C_2 & \text{if } n = 1, \end{cases} \tag{4.21}$$

where C_1 and C_2 are constants.

Note that $\lceil x \rceil$ stands for the smallest integer larger than or equal to x, while $\lfloor x \rfloor$ stands for the largest integer less than or equal to x. It turns out that the solution to (4.20) and (4.21) are roughly the same, in a sense that will hopefully become clear later. (This is almost always the case.) For now, let us not worry about floors and ceilings and the distinction between things that take 1 unit of time and things that take no more than some constant amount of time.

Let's turn to another example of a divide and conquer algorithm, *mergesort*. In this algorithm, you wish to sort a list of n items. Let us assume that the data is stored in an array A in positions 1 through n. Mergesort can be described as follows:

```
MergeSort(A,low,high)
     if (low == high)
          return
     else
          mid = (low + high)/2
          MergeSort(A,low,mid)
          MergeSort(A,mid+1,high)
          Merge the sorted lists from the previous two steps
```

More details on mergesort can be found in almost any algorithms textbook. Suffice to say that the base case (low = high) takes one step, while the other case executes 1 step, makes two recursive calls on problems of size $n/2$, and then executes the Merge instruction, which can be done in n steps.

Thus we obtain the following recurrence for the running time of mergesort:

$$T(n) = \begin{cases} 2T(n/2) + n & \text{if } n > 1 \\ 1 & \text{if } n = 1 \end{cases} \tag{4.22}$$

Recurrences such as this one can be understood via the idea of a recursion tree, which we introduce below. This concept allows us to analyze recurrences that arise in divide-and-conquer algorithms, and those that arise in other recursive situations, such as the Towers of Hanoi, as well. A recursion tree for a recurrence is a visual and conceptual representation of the process of iterating the recurrence.

Recursion Trees

We will introduce the idea of a recursion tree via several examples. It is helpful to have an "algorithmic" interpretation of a recurrence. For example, (ignoring for a moment the base case) we can interpret the recurrence

$$T(n) = 2T(n/2) + n \tag{4.23}$$

as "in order to solve a problem of size n we must solve 2 problems of size $n/2$ and do n units of additional work." Similarly we can interpret

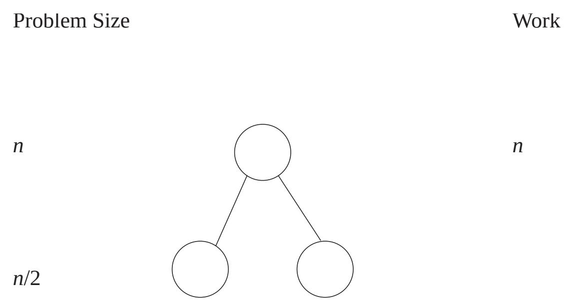
$$T(n) = T(n/4) + n^2$$

as "in order to solve a problem of size n we must solve one problem of size $n/4$ and do n^2 units of additional work."

We can also interpret the recurrence

$$T(n) = 3T(n-1) + n$$

Figure 4.2: The initial stage of drawing a recursion tree diagram.



as "in order to solve a problem of size n, we must solve 3 subproblems of size $n-1$ and do n additional units of work.

In Figure 4.2 we draw the beginning of the recursion tree diagram for (4.23). For now, assume n is a power of 2. A recursion tree diagram has three parts, a left, a middle, and a right. On the left, we keep track of the problem size, in the middle we draw the tree, and on right we keep track of the work done. We draw the diagram in levels, each level of the diagram representing a level of recursion. Equivalently, each level of the diagram represents a level of iteration of the recurrence. So to begin the recursion tree for (4.23), we show, in level 0 on the left, that we have problem of size n. Then by drawing a root vertex with two edges leaving it, we show in the middle that we are splitting our problem into 2 problems. We note on the right that we do n units of work in addition to whatever is done on the two new problems we created. In the next level, we draw two vertices in the middle representing the two problems into which we split our main problem and show on the left that each of these problems has size $n/2$.

You can see how the recurrence is reflected in levels 0 and 1 of the recursion tree. The top vertex of the tree represents $T(n)$, and on the next level we have two problems of size $n/2$, representing the recursive term $2T(n/2)$ of our recurrence. Then after we solve these two problems we return to level 0 of the tree and do n additional units of work for the nonrecursive term of the recurrence.

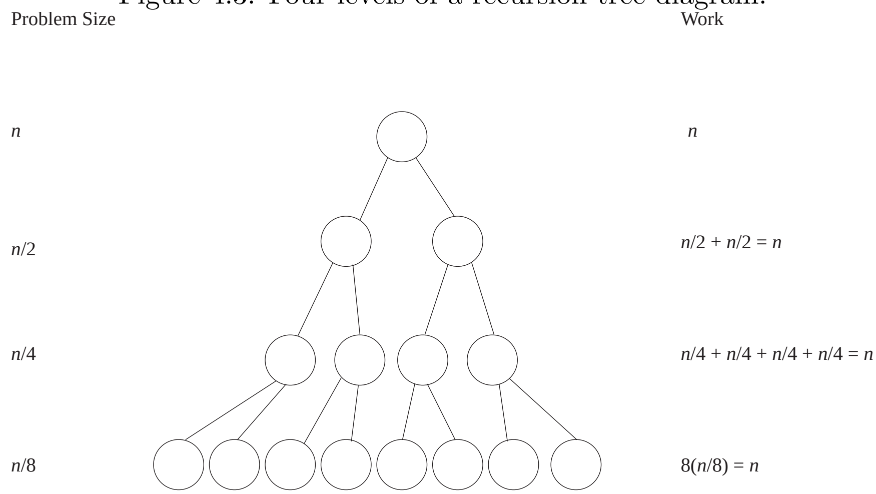
Now we continue to draw the tree in the same manner. Filling in the rest of level one and adding a few more levels, we get Figure 4.3.

Let us summarize what the diagram tells us so far. At level zero (the top level), n units of work are done. We see that at each succeeding level, we halve the problem size and double the number of subproblems. We also see that at level 1, each of the two subproblems requires $n/2$ units of additional work, and so a total of n units of additional work are done. Similarly level 2 has 4 subproblems of size $n/4$ and so $4(n/4) = n$ units of additional work are done. Notice that to compute the total work done on a level we multiply the number of subproblems by the amount of additional work per subproblem.

To see how iteration of the recurrence is reflected in the diagram, we iterate the recurrence once, getting

$$
\begin{aligned}
T(n) &= 2T(n/2) + n \\
T(n) &= 2(2T(n/4) + n/2) + n \\
T(n) &= 4T(n/4) + n + n = 4T(n/4) + 2n
\end{aligned}
$$

Figure 4.3: Four levels of a recursion tree diagram.



If we examine levels 0, 1, and 2 of the diagram, we see that at level 2 we have four vertices which represent four problems, each of size $n/4$ This corresponds to the recursive term that we obtained after iterating the recurrence. However after we solve these problems we return to level 1 where we twice do $n/2$ additional units of work and to level 0 where we do another n additional units of work. In this way each time we add a level to the tree we are showing the result of one more iteration of the recurrence.

We now have enough information to be able to describe the recursion tree diagram in general. To do this, we need to determine, for each level, three things:

- the number of subproblems,
- the size of each subproblem,
- the total work done at that level.

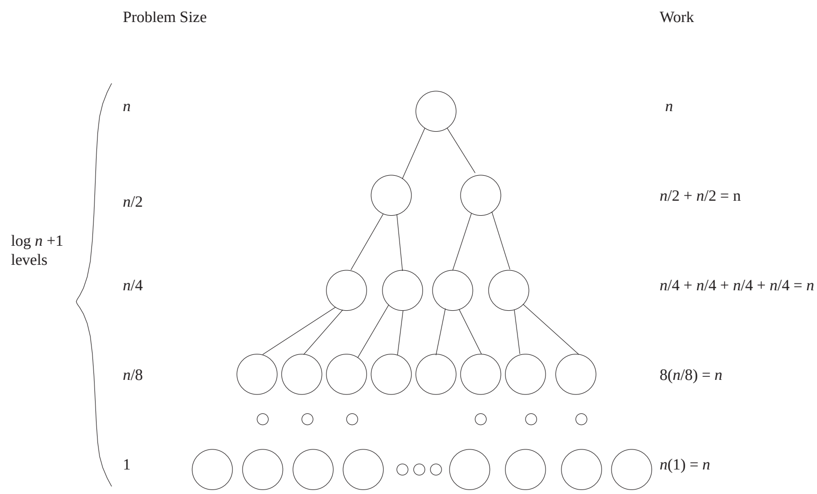
We also need to figure out how many levels there are in the recursion tree.

We see that for this problem, at level i, we have 2^i subproblems of size $n/2^i$. Further, since a problem of size 2^i requires 2^i units of additional work, there are $(2^i)[n/(2^i)] = n$ units of work done per level. To figure out how many levels there are in the tree, we just notice that at each level the problem size is cut in half, and the tree stops when the problem size is 1. Therefore there are $\log_2 n + 1$ levels of the tree, since we start with the top level and cut the problem size in half $\log_2 n$ times.[2] We can thus visualize the whole tree in Figure 4.4.

The computation of the work done at the bottom level is different from the other levels. In the other levels, the work is described by the recursive equation of the recurrence; in this case the amount of work is the n in $T(n) = 2T(n/2) + n$. At the bottom level, the work comes from the base case. Thus we must compute the number of problems of size 1 (assuming that one is the base case), and then multiply this value by $T(1) = 1$. In our recursion tree in Figure 4.4, the number of nodes at the bottom level is $2^{\log_2 n} = n$. Since $T(1) = 1$, we do n units of work at

[2] To simplify notation, for the remainder of the book, if we omit the base of a logarithm, it should be assumed to be base 2.

Figure 4.4: A finished recursion tree diagram.



the bottom level of the tree. Had we chosen to say that $T(1)$ was some constant other than 1, this would not have been the case. We emphasize that the correct value always comes from the base case; it is just a coincidence that it sometimes also comes from the recursive equation of the recurrence.

The bottom level of the tree represents the final stage of iterating the recurrence. We have seen that at this level we have n problems each requiring work $T(1) = 1$, giving us total work n at that level. After we solve the problems represented by the bottom level, we have to do all the additional work from all the earlier levels. For this reason, we sum the work done at all the levels of the tree to get the total work done. *Iteration of the recurrence shows us that the solution to the recurrence is the sum of all the work done at all the levels of the recursion tree.*

The important thing is that we now know how much work is done at each level. Once we know this, we can sum the total amount of work done over all the levels, giving us the solution to our recurrence. In this case, there are $\log_2 n + 1$ levels, and at each level the amount of work we do is n units. Thus we conclude that the total amount of work done to solve the problem described by recurrence (4.23) is $n(\log_2 n + 1)$. The total work done throughout the tree is the solution to our recurrence, because the tree simply models the process of iterating the recurrence. Thus the solution to recurrence (4.22) is $T(n) = n(\log n + 1)$.

Since one unit of time will vary from computer to computer, and since some kinds of work might take longer than other kinds, we are usually interested in the big-θ behavior of $T(n)$. For example, we can consider a recurrence that it identical to (4.22), except that $T(1) = a$, for some constant a. In this case, $T(n) = an + n \log n$, because an units of work are done at level 1 and n additional units of work are done at each of the remaining $\log n$ levels. It is still true that $T(n) = \Theta(n \log n)$, because the different base case did not change the solution to the recurrence by more than a constant factor[3]. Although recursion trees can give us the exact solutions (such as $T(n) = an + n \log n$ above) to recurrences, our interest in the big-Θ behavior of solutions will usually lead us to use a recursion tree to determine the big-Θ or even, in complicated cases, just the big-O behavior of the actual solution to the recurrence. In Problem 10 we explore whether

[3]More precisely, $n \log n < an + n \log n < (a + 1)n \log n$ for any $a > 0$.

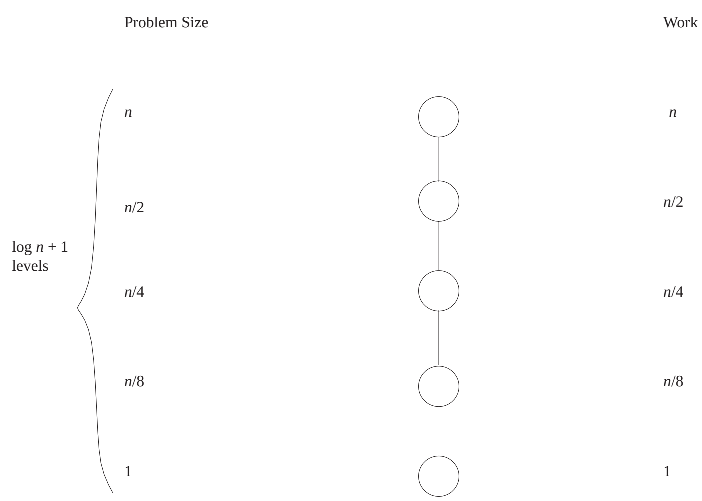
the value of $T(1)$ actually influences the big-Θ behavior of the solution to a recurrence.

Let's look at one more recurrence.

$$T(n) = \begin{cases} T(n/2) + n & \text{if } n > 1 \\ 1 & \text{if } n = 1 \end{cases} \tag{4.24}$$

Again, assume n is a power of two. We can interpret this as follows: to solve a problem of size n, we must solve one problem of size $n/2$ and do n units of additional work. We draw the tree for this problem in Figure 4.5 and see that the problem sizes are the same as in the previous tree. The remainder, however, is different. The number of subproblems does not double, rather

Figure 4.5: A recursion tree diagram for Recurrence 4.24.



it remains at one on each level. Consequently the amount of work halves at each level. Note that there are still $\log n + 1$ levels, as the number of levels is determined by how the problem size is changing, not by how many subproblems there are. So on level i, we have 1 problem of size $n/2^i$, for total work of $n/2^i$ units.

We now wish to compute how much work is done in solving a problem that gives this recurrence. Note that the additional work done is different on each level, so we have that the total amount of work is

$$n + n/2 + n/4 + \cdots + 2 + 1 = n\left(1 + \frac{1}{2} + \frac{1}{4} + \cdots + \left(\frac{1}{2}\right)^{\log_2 n}\right),$$

which is n times a geometric series. By Theorem 4.4, the value of a geometric series in which the largest term is one is $\Theta(1)$. This implies that the work done is described by $T(n) = \Theta(n)$.

We emphasize that there is exactly one solution to recurrence (4.24); it is the one we get by using the recurrence to compute $T(2)$ from $T(1)$, then to compute $T(4)$ from $T(2)$, and so on. What we have done here is show that $T(n) = \Theta(n)$. In fact, for the kinds of recurrences we have been examining, once we know $T(1)$ we can compute $T(n)$ for any relevant n by repeatedly using the recurrence, so there is no question that solutions do exist and can, in principle, be computed for any value of n. In most applications, we are not interested in the exact form of the solution, but a big-O upper bound, or Big-Θ bound on the solution.

Exercise 4.3-2 Find a big-Θ bound for the solution to the recurrence

$$T(n) = \begin{cases} 3T(n/3) + n & \text{if } n \geq 3 \\ 1 & \text{if } n < 3 \end{cases}$$

using a recursion tree. Assume that n is a power of 3.

Exercise 4.3-3 Solve the recurrence

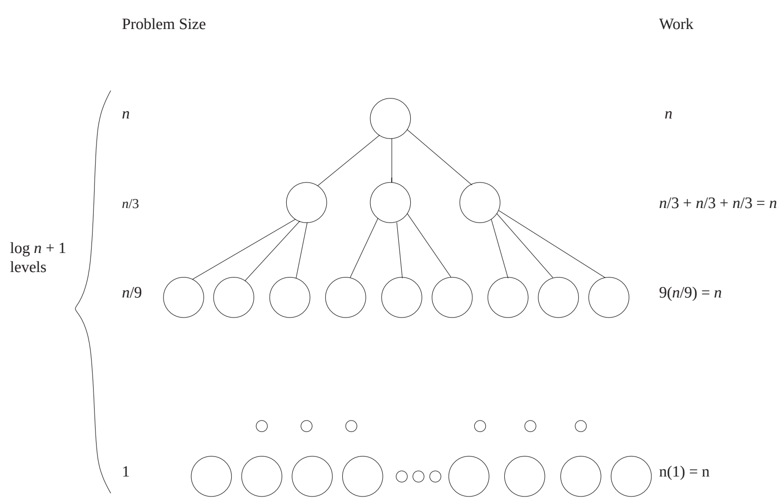
$$T(n) = \begin{cases} 4T(n/2) + n & \text{if } n \geq 2 \\ 1 & \text{if } n = 1 \end{cases}$$

using a recursion tree. Assume that n is a power of 2. Convert your solution to a big-Θ statement about the behavior of the solution.

Exercise 4.3-4 Can you give a general big-Θ bound for solutions to recurrences of the form $T(n) = aT(n/2) + n$ when n is a power of 2? You may have different answers for different values of a.

The recurrence in Exercise 4.3-2 is similar to the mergesort recurrence. One difference is that at each step we divide into 3 problems of size $n/3$. Thus we get the picture in Figure 4.6. Another difference is that the number of levels, instead of being $\log_2 n + 1$ is now $\log_3 n + 1$, so

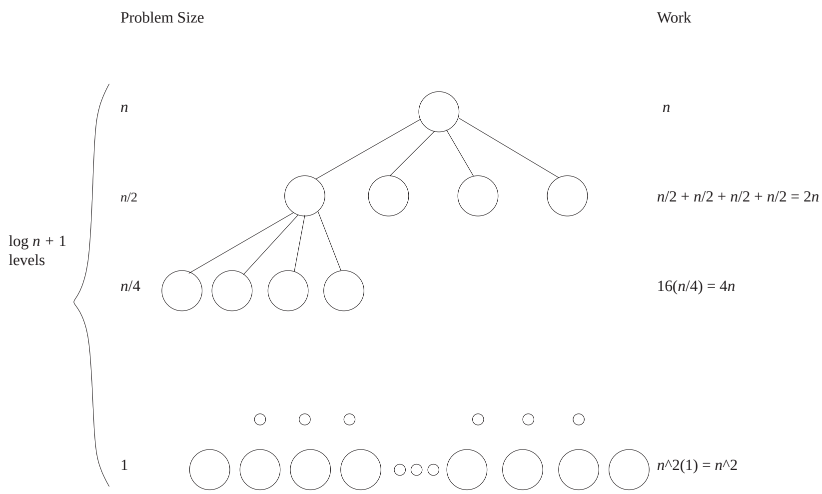
Figure 4.6: The recursion tree diagram for the recurrence in Exercise 4.3-2.



the total work is still $\Theta(n \log n)$ units. (Note that $\log_b n = \Theta(\log_2 n)$ for any $b > 1$.)

Now let's look at the recursion tree for Exercise 4.3-3. Here we have 4 children of size $n/2$, and we get Figure 4.7. Let's look carefully at this tree. Just as in the mergesort tree there are $\log_2 n + 1$ levels. However, in this tree, each node has 4 children. Thus level 0 has 1 node, level 1 has 4 nodes, level 2 has 16 nodes, and in general level i has 4^i nodes. On level i each node corresponds to a problem of size $n/2^i$ and hence requires $n/2^i$ units of additional work. Thus the total work on level i is $4^i(n/2^i) = 2^i n$ units. This formula applies on level $\log_2 n$ (the bottom

Figure 4.7: The Recursion tree for Exercise 4.3-3.



level) as well since there are $n^2 = 2^{\log_2 n} n$ nodes, each requiring $T(1) = 1$ work. Summing over the levels, we get

$$\sum_{i=0}^{\log_2 n} 2^i n = n \sum_{i=0}^{\log_2 n} 2^i.$$

There are many ways to simplify that expression, for example from our formula for the sum of a geometric series we get

$$\begin{aligned} T(n) &= n \sum_{i=0}^{\log_2 n} 2^i \\ &= n \frac{1 - 2^{(\log_2 n)+1}}{1-2} \\ &= n \frac{1-2n}{-1} \\ &= 2n^2 - n \\ &= \Theta(n^2). \end{aligned}$$

More simply, by Theorem 4.4 we have that $T(n) = n\Theta(2^{\log n}) = \Theta(n^2)$.

Three Different Behaviors

Now let's compare the recursion tree diagrams for the recurrences $T(n) = 2T(n/2) + n$, $T(n) = T(n/2) + n$ and $T(n) = 4T(n/2) + n$. Note that all three trees have depth $1 + \log_2 n$, as this is determined by the size of the subproblems relative to the parent problem, and in each case, the size of each subproblem is 1/2 the size of of the parent problem. The trees differ, however, in the amount of work done per level. In the first case, the amount of work on each level is the same. In the second case, the amount of work done on a level decreases as you go down the tree, with the most work being at the top level. In fact, it decreases geometrically, so by Theorem 4.4 the total work done is bounded above and below by a constant times the work done at the root node. In the third case, the number of nodes per level is growing at a faster rate than the problem size is decreasing, and the level with the largest amount of work is the bottom one. Again we have a geometric series, and so by Theorem 4.4 the total work is bounded above and below by a constant times the amount of work done at the last level.

If you understand these three cases and the differences among them, you now understand the great majority of the recursion trees that arise in algorithms.

So to answer Exercise 4.3-4, which asks for a general Big-Θ bound for the solutions to recurrences of the form $T(n) = aT(n/2) + n$, we can conclude the following:

Lemma 4.7 *Suppose that we have a recurrence of the form*

$$T(n) = aT(n/2) + n,$$

where a is a positive integer and $T(1)$ is nonnegative. Thus we have the following big-Theta bounds on the solution.

1. *If $a < 2$ then $T(n) = \Theta(n)$.*
2. *If $a = 2$ then $T(n) = \Theta(n \log n)$*
3. *If $a > 2$ then $T(n) = \Theta(n^{\log_2 a})$*

Proof: Cases 1 and 2 follow immediately from our observations above. We can verify case 3 as follows. At each level i we have a^i nodes, each corresponding to a problem of size $n/2^i$. Thus at level i the total amount of work is $a^i(n/2^i) = n(a/2)^i$ units. Summing over the $\log_2 n$ levels, we get

$$a^{\log_2 n}T(1) + n \sum_{i=0}^{(\log_2 n)-1} (a/2)^i.$$

The sum given by the summation sign is a geometric series, so, since $a/2 \neq 1$, the sum will be big-Θ of the largest term (see Theorem 4.4). Since $a > 2$, the largest term in this case is clearly the last one, namely $n(a/2)^{(\log_2 n)-1}$, and applying rules of exponents and logarithms, we get that n times the largest term is

$$\begin{aligned} n\left(\frac{a}{2}\right)^{(\log_2 n)-1} &= \frac{2}{a} \cdot \frac{n \cdot a^{\log_2 n}}{2^{\log_2 n}} = \frac{2}{a} \cdot \frac{n \cdot a^{\log_2 n}}{n} = \frac{2}{a} \cdot a^{\log_2 n} \\ &= \frac{2}{a} a^{\log_2 (a^{log_2 a}} = \frac{2}{a} \cdot 2^{\log_2 a \log_2 n} = \frac{2}{a} \cdot n^{\log_2 a}. \end{aligned} \tag{4.25}$$

Thus $T(1)a^{\log_2 n} = T(1)n^{\log_2 a}$. Since $\frac{2}{a}$ and $T(1)$ are both nonnegative, the total work done is $\Theta(n^{\log_2 a})$. ■

In fact Lemma 4.7 holds for all positive real numbers a; we can iterate the recurrence to see this. Since a recursion tree diagram is a way to visualize iterating the recurrence when a is an integer, iteration is the natural thing to try when a is not an integer.

Notice that in the last two equalities of computation we made in Equation 4.25, we showed that $a^{\log n} = n^{\log a}$. This is a useful and, perhaps, surprising fact, so we state it (in slightly more generality) as a corollary to the proof.

Corollary 4.8 *For any base b, we have $a^{\log_b n} = n^{\log_b a}$.*

Important Concepts, Formulas, and Theorems

1. *Divide and Conquer Algorithm.* A *divide and conquer algorithm* is one that solves a problem by dividing it into problems that are smaller but otherwise of the same type as the original one, recursively solves these problems, and then assembles the solution of these so-called subproblems into a solution of the original one. Not all problems can be solved by such a strategy, but a great many problems of interest in computer science can.

2. *Mergesort.* In *mergesort* we sort a list of items that have some underlying order by dividing the list in half, sorting the first half (by recursively using mergesort), sorting the second half (by recursively using mergesort), and then merging the two sorted list. For a list of length one mergesort returns the same list.

3. *Recursion Tree.* A *recursion tree diagram* for a recurrence of the form $T(n) = aT(n/b)+g(n)$ has three parts, a left, a middle, and a right. On the left, we keep track of the problem size, in the middle we draw the tree, and on right we keep track of the work done. We draw the diagram in levels, each level of the diagram representing a level of recursion. The tree has a vertex representing the initial problem and one representing each subproblem we have to solve. Each non-leaf vertex has a children. The vertices are divided into levels corresponding to (sub-)problems of the same size; to the left of a level of vertices we write the size of the problems the vertices correspond to; to the right of the vertices on a given level we write the total amount of work done at that level by an algorithm whose work is described by the recurrence, not including the work done by any recursive calls from that level.

4. *The Base Level of a Recursion Tree.* The amount of work done on the lowest level in a recursion tree is the number of nodes times the value given by the initial condition; it is not determined by attempting to make a computation of "additional work" done at the lowest level.

5. *Bases for Logarithms.* We use $\log n$ as an alternate notation for $\log_2 n$. A fundamental fact about logarithms is that $\log_b n = \Theta(\log_2 n)$ for any real number $b > 1$.

6. *An Important Fact About Logarithms.* For any $b > 0$, $a^{\log_b n} = n^{\log_b a}$.

7. *Three behaviors of solutions.* The solution to a recurrence of the form $T(n) = aT(n/2) + n$ behaves in one of the following ways:

   (a) if $a < 2$ then $T(n) = \Theta(n)$.

   (b) if $a = 2$ then $T(n) = \Theta(n \log n)$

   (c) if $a > 2$ then $T(n) = \Theta(n^{\log_2 a})$.

Problems

1. Draw recursion trees and find big-Θ bounds on the solutions to the following recurrences. For all of these, assume that $T(1) = 1$ and n is a power of the appropriate integer.

   (a) $T(n) = 8T(n/2) + n$

   (b) $T(n) = 8T(n/2) + n^3$

(c) $T(n) = 3T(n/2) + n$
(d) $T(n) = T(n/4) + 1$
(e) $T(n) = 3T(n/3) + n^2$

2. Draw recursion trees and find exact solutions to the following recurrences. For all of these, assume that $T(1) = 1$ and n is a power of the appropriate integer.

   (a) $T(n) = 8T(n/2) + n$
   (b) $T(n) = 8T(n/2) + n^3$
   (c) $T(n) = 3T(n/2) + n$
   (d) $T(n) = T(n/4) + 1$
   (e) $T(n) = 3T(n/3) + n^2$

3. Find the exact solution to Recurrence 4.24.

4. Show that $\log_b n = \Theta(\log_2 n)$, for any constant $b > 1$.

5. Prove Corollary 4.8 by showing that $a^{\log_b n} = n^{\log_b a}$ for any $b > 0$.

6. Recursion trees will still work, even if the problems do not break up geometrically, or even if the work per level is not n^c units. Draw recursion trees and and find the best big-O bounds you can for solutions to the following recurrences. For all of these, assume that $T(1) = 1$.

   (a) $T(n) = T(n-1) + n$
   (b) $T(n) = 2T(n-1) + n$
   (c) $T(n) = T(\lfloor\sqrt{n}\rfloor) + 1$ (You may assume n has the form $n = 2^{2^i}$.)
   (d) $T(n) = 2T(n/2) + n\log n$ (You may assume n is a power of 2.)

7. In each case in the previous problem, is the big-O bound you found a big-Θ bound?

8. If $S(n) = aS(n-1) + g(n)$ and $g(n) < c^n$ with $0 \le c < a$, how fast does $S(n)$ grow (in big-Θ terms)?

9. If $S(n) = aS(n-1) + g(n)$ and $g(n) = c^n$ with $0 < a \le c$, how fast does $S(n)$ grow in big-Θ terms?

10. Given a recurrence of the form $T(n) = aT(n/b) + g(n)$ with $T(1) = c > 0$ and $g(n) > 0$ for all n and a recurrence of the form $S(n) = aS(n/b) + g(n)$ with $S(1) = 0$ (and the same a, b, and $g(n)$), is there any difference in the big-Θ behavior of the solutions to the two recurrences? What does this say about the influence of the initial condition on the big-Θ behavior of such recurrences?

4.4 The Master Theorem

Master Theorem

In the last section, we saw three different kinds of behavior for recurrences of the form

$$T(n) = \begin{cases} aT(n/2) + n & \text{if } n > 1 \\ d & \text{if } n = 1. \end{cases}$$

These behaviors depended upon whether $a < 2$, $a = 2$, or $a > 2$. Remember that a was the number of subproblems into which our problem was divided. Dividing by 2 cut our problem size in half each time, and the n term said that after we completed our recursive work, we had n additional units of work to do for a problem of size n. There is no reason that the amount of additional work required by each subproblem needs to be the size of the subproblem. In many applications it will be something else, and so in Theorem 4.9 we consider a more general case. Similarly, the sizes of the subproblems don't have to be 1/2 the size of the parent problem. We then get the following theorem, our first version of a theorem called the *Master Theorem.* (Later on we will develop some stronger forms of this theorem.)

Theorem 4.9 *Let a be an integer greater than or equal to* 1 *and b be a real number greater than* 1*. Let c be a positive real number and d a nonnegative real number. Given a recurrence of the form*

$$T(n) = \begin{cases} aT(n/b) + n^c & \textit{if } n > 1 \\ d & \textit{if } n = 1 \end{cases}$$

in which n is restricted to be a power of b,

1. *if* $\log_b a < c$, $T(n) = \Theta(n^c)$,
2. *if* $\log_b a = c$, $T(n) = \Theta(n^c \log n)$,
3. *if* $\log_b a > c$, $T(n) = \Theta(n^{\log_b a})$.

Proof: In this proof, we will set $d = 1$, so that the work done at the bottom level of the tree is the same as if we divided the problem one more time and used the recurrence to compute the additional work. As in Footnote 3 in the previous section, it is straightforward to show that we get the same big-Θ bound if d is positive. It is only a little more work to show that we get the same big-Θ bound if d is zero.

Let's think about the recursion tree for this recurrence. There will be $1 + \log_b n$ levels. At each level, the number of subproblems will be multiplied by a, and so the number of subproblems at level i will be a^i. Each subproblem at level i is a problem of size (n/b^i). A subproblem of size n/b^i requires $(n/b^i)^c$ additional work and since there are a^i problems on level i, the total number of units of work on level i is

$$a^i(n/b^i)^c = n^c \left(\frac{a^i}{b^{ci}}\right) = n^c \left(\frac{a}{b^c}\right)^i. \tag{4.26}$$

Recall from Lemma 4.7 that the different cases for $c = 1$ were when the work per level was decreasing, constant, or increasing. The same analysis applies here. From our formula for work on level i, we see that the work per level is decreasing, constant, or increasing exactly when $(\frac{a}{b^c})^i$ is decreasing, constant, or increasing, respectively. These three cases depend on whether $(\frac{a}{b^c})$ is less than one, equal to one, or greater than one, respectively. Now observe that

$$\begin{array}{rc} & (\frac{a}{b^c}) = 1 \\ \Leftrightarrow & a = b^c \\ \Leftrightarrow & \log_b a = c \log_b b \\ \Leftrightarrow & \log_b a = c. \end{array}$$

This shows us where the three cases in the statement of the theorem come from. Now we need to show the bound on $T(n)$ in the different cases. In the following paragraphs, we will use the facts (whose proof is a straightforward application of the definition of logarithms and rules of exponents) that for any x, y and z, each greater than 1, $x^{\log_y z} = z^{\log_y x}$ (see Corollary 4.8, Problem 5 at the end of the previous section, and Problem 3 at the end of this section) and that $\log_x y = \Theta(\log_2 y)$ (see Problem 4 at the end of the previous section).

In general, the total work done is computed by summing the expression for the work per level given in Equation 4.26 over all the levels, giving

$$\sum_{i=0}^{\log_b n} n^c \left(\frac{a}{b^c}\right)^i = n^c \sum_{i=0}^{\log_b n} \left(\frac{a}{b^c}\right)^i$$

In case 1, (part 1 in the statement of the theorem) this is n^c times a geometric series with a ratio of less than 1. Theorem 4.4 tells us that

$$n^c \sum_{i=0}^{\log_b n} \left(\frac{a}{b^c}\right)^i = \Theta(n^c).$$

Exercise 4.4-1 Prove Case 2 (part 2 of the statement) of the Master Theorem.

Exercise 4.4-2 Prove Case 3 (part 3 of the statement) of the Master Theorem.

In Case 2 we have that $\frac{a}{b^c} = 1$ and so

$$\begin{aligned} n^c \sum_{i=0}^{\log_b n} \left(\frac{a}{b^c}\right)^i &= n^c \sum_{i=0}^{\log_b n} 1^i \\ &= n^c(1 + \log_b n) \\ &= \Theta(n^c \log n). \end{aligned}$$

In Case 3, we have that $\frac{a}{b^c} > 1$. So in the series

$$\sum_{i=0}^{\log_b n} n^c \left(\frac{a}{b^c}\right)^i = n^c \sum_{i=0}^{\log_b n} \left(\frac{a}{b^c}\right)^i,$$

the largest term is the last one, so by Theorem 4.4,the sum is $\Theta\left(n^c \left(\frac{a}{b^c}\right)^{\log_b n}\right)$. But

$$
\begin{aligned}
n^c\left(\frac{a}{b^c}\right)^{\log_b n} &= n^c \cdot \frac{a^{\log_b n}}{(b^c)^{\log_b n}} \\
&= n^c \cdot \frac{n^{\log_b a}}{n^{\log_b b^c}} \\
&= n^c \cdot \frac{n^{\log_b a}}{n^c} \\
&= n^{\log_b a}.
\end{aligned}
$$

Thus the solution is $\Theta(n^{\log_b a})$. ■

We note that we may assume that a is a real number with $a > 1$ and give a somewhat similar proof (replacing the recursion tree with an iteration of the recurrence), but we do not give the details here.

Solving More General Kinds of Recurrences

Exercise 4.4-3 What can you say about the big-θ behavior of the solution to

$$
T(n) = \begin{cases} 2T(n/3) + 4n^{3/2} & \text{if } n > 1 \\ d & \text{if } n = 1, \end{cases}
$$

where n can be any nonnegative power of three?

Exercise 4.4-4 If $f(n) = n\sqrt{n+1}$, what can you say about the Big-Θ behavior of solutions to

$$
S(n) = \begin{cases} 2S(n/3) + f(n) & \text{if } n > 1 \\ d & \text{if } n = 1, \end{cases}
$$

where n can be any nonnegative power of three?

For Exercise 4.4-3, the work done at each level of the tree except for the bottom level will be four times the work done by the recurrence

$$
T'(n) = \begin{cases} 2T'(n/3) + n^{3/2} & \text{if } n > 1 \\ d & \text{if } n = 1, \end{cases}
$$

Thus the work done by T will be no more than four times the work done by T', but will be larger than the work done by T'. Therefore $T(n) = \Theta(T'(n))$. Thus by the master theorem, since $\log_3 2 < 1 < 3/2$, we have that $T(n) = \Theta(n^{3/2})$.

For Exercise 4.4-4, Since $n\sqrt{n+1} > n\sqrt{n} = n^{3/2}$ we have that $S(n)$ is at least as big as the solution to the recurrence

$$
T'(n) = \begin{cases} 2T'(n/3) + n^{3/2} & \text{if } n > 1 \\ d & \text{if } n = 1, \end{cases}
$$

where n can be any nonnegative power of three. But the solution to the recurrence for S will be no more than the solution to the recurrence in Exercise 4.4-3 for T, because $n\sqrt{n+1} \leq 4n^{3/2}$ for $n \geq 0$. Since $T(n) = \Theta(T'(n))$, then $S(n) = \Theta(T'(n))$ as well.

Extending the Master Theorem

As Exercise 4.4-3 and Exercise 4.4-4 suggest, there is a whole range of interesting recurrences that do not fit the master theorem but are closely related to recurrences that do. These recurrences have the same kind of behavior predicted by our original version of the Master Theorem, but the original version of the Master Theorem does not apply to them, just as it does not apply to the recurrences of Exercise 4.4-3 and Exercise 4.4-4.

We now state a second version of the Master Theorem that covers these cases. A still stronger version of the theorem may be found in *Introduction to Algorithms* by Cormen, et. al., but the version here captures much of the interesting behavior of recurrences that arise from the analysis of algorithms.

Theorem 4.10 *Let a and b be positive real numbers with $a \geq 1$ and $b > 1$. Let $T(n)$ be defined for powers n of b by*

$$T(n) = \begin{cases} aT(n/b) + f(n) & \text{if } n > 1 \\ d & \text{if } n = 1. \end{cases}$$

Then

1. *if $f(n) = \Theta(n^c)$ where $\log_b a < c$, then $T(n) = \Theta(n^c) = \Theta(f(n))$.*
2. *if $f(n) = \Theta(n^c)$, where $\log_b a = c$, then $T(n) = \Theta(n^{\log_b a} \log_b n)$*
3. *if $f(n) = \Theta(n^c)$, where $\log_b a > c$, then $T(n) = \Theta(n^{\log_b a})$.*

Proof: We construct a recursion tree or iterate the recurrence. Since we have assumed that $f(n) = \Theta(n^c)$, there are constants c_1 and c_2, independent of the level, so that the work at each level is between $c_1 n^c \left(\frac{a}{b^c}\right)^i$ and $c_2 n^c \left(\frac{a}{b^c}\right)^i$ so from this point on the proof is largely a translation of the original proof. ■

Exercise 4.4-5 What does the Master Theorem tell us about the solutions to the recurrence

$$T(n) = \begin{cases} 3T(n/2) + n\sqrt{n+1} & \text{if } n > 1 \\ 1 & \text{if } n = 1? \end{cases}$$

As we saw in our solution to Exercise 4.4-4 $x\sqrt{x+1} = \Theta(x^{3/2})$. Since $2^{3/2} = \sqrt{2^3} = \sqrt{8} < 3$, we have that $\log_2 3 > 3/2$. Then by conclusion 3 of version 2 of the Master Theorem, $T(n) = \Theta(n^{\log_2 3})$.

The remainder of this section is devoted to carefully analyzing divide and conquer recurrences in which n is not a power of b and $T(n/b)$ is replaced by $T(\lceil n/b \rceil)$. While the details are somewhat technical, the end result is that the big-Θ behavior of such recurrences is the same as the corresponding recurrences for functions defined on powers of b. In particular, the following theorem is a consequence of what we prove.

Theorem 4.11 *Let a and b be positive real numbers with $a \geq 1$ and $b \geq 2$. Let $T(n)$ satisfy the recurrence*

$$T(n) = \begin{cases} aT(\lceil n/b \rceil) + f(n) & \text{if } n > 1 \\ d & \text{if } n = 1. \end{cases}$$

Then

1. *if $f(n) = \Theta(n^c)$ where $\log_b a < c$, then $T(n) = \Theta(n^c) = \Theta(f(n))$.*
2. *if $f(n) = \Theta(n^c)$, where $\log_b a = c$, then $T(n) = \Theta(n^{\log_b a} \log_b n)$*
3. *if $f(n) = \Theta(n^c)$, where $\log_b a > c$, then $T(n) = \Theta(n^{\log_b a})$.*

(The condition that $b \geq 2$ can be changed to $B > 1$ with an appropriate change in the base case of the recurrence, but the base case will then depend on b.) The reader should be able to skip over the remainder of this section without loss of continuity.

More realistic recurrences (Optional)

So far, we have considered divide and conquer recurrences for functions $T(n)$ defined on integers n which are powers of b. In order to consider a more realistic recurrence in the master theorem, namely

$$T(n) = \begin{cases} aT(\lceil n/b \rceil) + n^c & \text{if } n > 1 \\ d & \text{if } n = 1, \end{cases}$$

or

$$T(n) = \begin{cases} aT(\lfloor n/b \rfloor) + n^c & \text{if } n > 1 \\ d & \text{if } n = 1, \end{cases}$$

or even

$$T(n) = \begin{cases} a'T(\lceil n/b \rceil) + (a - a')T(\lfloor n/b \rfloor) + n^c & \text{if } n > 1 \\ d & \text{if } n = 1, \end{cases}$$

it turns out to be easiest to first extend the domain for our recurrences to a much bigger set than the nonnegative integers, either the real or rational numbers, and then to work backwards.

For example, we can write a recurrence of the form

$$t(x) = \begin{cases} f(x)t(x/b) + g(x) & \text{if } x \geq b \\ k(x) & \text{if } 1 \leq x < b \end{cases}$$

for two (known) functions f and g defined on the real [or rational] numbers greater than 1 and one (known) function k defined on the real [or rational] numbers x with $1 \leq x < b$. Then so long as $b > 1$ it is possible to prove that there is a unique function t defined on the real [or rational] numbers greater than or equal to 1 that satisfies the recurrence. We use the lower case t in this situation as a signal that we are considering a recurrence whose domain is the real or rational numbers greater than or equal to 1.

Exercise 4.4-6 How would we compute $t(x)$ in the recurrence

$$t(x) = \begin{cases} 3t(x/2) + x^2 & \text{if } x \geq 2 \\ 5x & \text{if } 1 \leq x < 2 \end{cases}$$

if x were 7? How would we show that there is one and only one function t that satisfies the recurrence?

Exercise 4.4-7 Is it the case that there is one and only one solution to the recurrence

$$T(n) = \begin{cases} f(n)T(\lceil n/b \rceil) + g(n) & \text{if } n > 1 \\ k & \text{if } n = 1 \end{cases}$$

when f and g are (known) functions defined on the positive integers, and k and b are (known) constants with b an integer larger than or equal to 2?

To compute $t(7)$ in Exercise 4.4-6 we need to know $t(7/2)$. To compute $t(7/2)$, we need to know $t(7/4)$. Since $1 < 7/4 < 2$, we know that $\mathrm{t}(7/4) = 35/4$. Then we may write

$$t(7/2) = 3 \cdot \frac{35}{4} + \frac{49}{4} = \frac{154}{4} = \frac{77}{2}.$$

Next we may write

$$\begin{aligned} t(7) &= 3t(7/2) + 7^2 \\ &= 3 \cdot \frac{77}{2} + 49 \\ &= \frac{329}{2}. \end{aligned}$$

Clearly we can compute $t(x)$ in this way for any x, though we are unlikely to enjoy the arithmetic. On the other hand suppose all we need to do is to show that there is a unique value of $t(x)$ determined by the recurrence, for all real numbers $x \geq 1$. If $1 \leq x < 2$, then $t(x) = 5x$, which uniquely determines $t(x)$. Given a number $x \geq 2$, there is a smallest integer i such that $x/2^i < 2$, and for this i, we have $1 \leq x/2^i$. We can now prove by induction on i that $t(x)$ is uniquely determined by the recurrence relation.

In Exercise 4.4-7 there is one and only one solution. Why? Clearly $T(1)$ is determined by the recurrence. Now assume inductively that $n > 1$ and that $T(m)$ is uniquely determined for positive integers $m < n$. We know that $n \geq 2$, so that $n/2 \leq n - 1$. Since $b \geq 2$, we know that $n/2 \geq n/b$, so that $n/b \leq n - 1$. Therefore $\lceil n/b \rceil < n$, so that we know by the inductive hypothesis that $T(\lceil n/b \rceil)$ is uniquely determined by the recurrence. Then by the recurrence,

$$T(n) = f(n)T\left(\left\lceil \frac{n}{b} \right\rceil\right) + g(n),$$

which uniquely determines $T(n)$. Thus by the principle of mathematical induction, $T(n)$ is determined for all positive integers n.

For every kind of recurrence we have dealt with, there is similarly one and only one solution. Because we know solutions exist, we don't find formulas for solutions to demonstrate that solutions exist, but rather to help us understand properties of the solutions. In this section and the last section, for example, we were interested in how fast the solutions grew as n grew large. This is why we were finding Big-O and Big-Θ bounds for our solutions.

Recurrences for general n (Optional)

We will now show how recurrences for arbitrary real numbers relate to recurrences involving floors and ceilings. We begin by showing that the conclusions of the Master Theorem apply to recurrences for arbitrary real numbers when we replace the real numbers by "nearby" powers of b.

Theorem 4.12 *Let a and b be positive real numbers with $b > 1$ and c and d be real numbers. Let $t(x)$ be the solution to the recurrence*

$$t(x) = \begin{cases} at(x/b) + x^c & \text{if } x \geq b \\ d & \text{if } 1 \leq x < b. \end{cases}$$

Let $T(n)$ be the solution to the recurrence

$$T(n) = \begin{cases} aT(n/b) + n^c & \text{if } n \geq 0 \\ d & \text{if } n = 1, \end{cases}$$

defined for n a nonnegative integer power of b. Let $m(x)$ be the largest integer power of b less than or equal to x. Then $t(x) = \Theta(T(m(x)))$

Proof: If we iterate (or, in the case that a is an integer, draw recursion trees for) the two recurrences, we can see that the results of the iterations are nearly identical. This means the solutions to the recurrences have the same big-Θ behavior. See the Appendix to this Section for details. ■

Removing Floors and Ceilings (Optional)

We have also pointed out that a more realistic Master Theorem would apply to recurrences of the form $T(n) = aT(\lfloor n/b \rfloor) + n^c$, or $T(n) = aT(\lceil n/b \rceil) + n^c$, or even $T(n) = a'T(\lceil n/b \rceil) + (a - a')T(\lfloor n/b \rfloor) + n^c$. For example, if we are applying mergesort to an array of size 101, we really break it into pieces, of size 50 and 51. Thus the recurrence we want is not really $T(n) = 2T(n/2) + n$, but rather $T(n) = T(\lfloor n/2 \rfloor) + T(\lceil n/2 \rceil) + n$.

We can show, however, that one can essentially "ignore" the floors and ceilings in typical divide-and-conquer recurrences. If we remove the floors and ceilings from a recurrence relation, we convert it from a recurrence relation defined on the integers to one defined on the rational numbers. However we have already seen that such recurrences are not difficult to handle.

The theorem below says that in recurrences covered by the master theorem, if we remove ceilings, our recurrences still have the same big-Θ bounds on their solutions. A similar proof shows that we may remove floors and still get the same big-Θ bounds. Without too much more work we can see that we can remove floors and ceilings simultaneously without changing the big-Θ bounds on our solutions. Since we may remove either floors or ceilings, that means that we may deal with recurrences of the form $T(n) = a'T(\lceil n/b \rceil) + (a - a')T(\lfloor n/b \rfloor) + n^c$. The condition that $b > 2$ can be replaced by $b > 1$, but the base case for the recurrence will depend on b.

Theorem 4.13 *Let a and b be positive real numbers with $b \geq 2$ and let c and d be real numbers. Let $T(n)$ be the function defined on the integers by the recurrence*

$$T(n) = \begin{cases} aT(\lceil n/b \rceil) + n^c & \text{if } n > 1 \\ d & n = 1, \end{cases}$$

and let $t(x)$ be the function on the real numbers defined by the recurrence

$$t(x) = \begin{cases} at(x/b) + x^c & \text{if } x \geq b \\ d & \text{if } 1 \leq x < b \end{cases}$$

Then $T(n) = \Theta(t(n))$. The same statement applies with ceilings replaced by floors.

Proof: As in the previous theorem, we can consider iterating the two recurrences. It is straightforward (though dealing with the notation is difficult) to show that for a given value of n, the iteration for computing $T(n)$ has at most two more levels than the iteration for computing $t(n)$. The work per level also has the same Big-Θ bounds at each level, and the work for the two additional levels of the iteration for $T(n)$ has the same Big-Θ bounds as the work at the bottom level of the recursion tree for $t(n)$. We give the details in the appendix at the end of this section. ■

Theorem 4.12 and Theorem 4.13 tell us that the Big-Θ behavior of solutions to our more realistic recurrences

$$T(n) = \begin{cases} aT(\lceil n/b \rceil) + n^c & \text{if } n > 1 \\ d & \text{n=1} \end{cases}$$

is determined by their Big-Θ behavior on powers of the base b.

Floors and ceilings in the stronger version of the Master Theorem (Optional)

In our first version of the master theorem, we showed that we could ignore ceilings and assume our variables were powers of b. In fact we can ignore them in circumstances where the function telling us the "work" done at each level of our recursion tree is $\Theta(x^c)$ for some positive real number c. This lets us apply the second version of the master theorem to recurrences of the form $T(n) = aT(\lceil n/b \rceil) + f(n)$.

Theorem 4.14 *Theorems 4.12 and 4.13 apply to recurrences in which the x^c or n^c term is replaced by $f(x)$ or $f(n)$ for a function f with $f(x) = \Theta(x^c)$.*

Proof: We iterate the recurrences or construct recursion trees in the same way as in the proofs of the original theorems, and find that the condition $f(x) = \Theta(x^c)$ gives us enough information to again bound the solution above and below with multiples of the solution of the recurrence with x^c. The details are similar to those in the original proofs. ■

Appendix: Proofs of Theorems (Optional)

For convenience, we repeat the statements of the earlier theorems whose proofs we merely outlined.

Theorem 4.12 *Let a and b be positive real numbers with $b > 1$ and c and d be real numbers. Let $t(x)$ be the solution to the recurrence*

$$t(x) = \begin{cases} at(x/b) + x^c & \text{if } x \geq b \\ d & \text{if } 1 \leq x < b. \end{cases}$$

Let $T(n)$ be the solution to the recurrence

$$T(n) = \begin{cases} aT(n/b) + n^c & \text{if } n \geq 0 \\ d & \text{if } n = 1, \end{cases}$$

defined for n is a nonnegative integer power of b. Let $m(x)$ be the largest integer power of b less than or equal to x. Then $t(x) = \Theta(T(m(x)))$

Proof: By iterating each recursion 4 times (or using a four level recursion tree in the case that a is an integer), we see that

$$t(x) = a^4 t\left(\frac{x}{b^4}\right) + \left(\frac{a}{b^c}\right)^3 x^c + \left(\frac{a}{b^c}\right)^2 x^c + \frac{a}{b^c} x^c$$

and

$$T(n) = a^4 T\left(\frac{n}{b^4}\right) + \left(\frac{a}{b^c}\right)^3 n^c + \left(\frac{a}{b^c}\right)^2 n^c + \frac{a}{b^c} n^c.$$

Thus, continuing until we have a solution, in both cases we get a solution that starts with a raised to an exponent that we will denote as either $e(x)$ or $e(n)$ when we want to distinguish between them and e when it is unnecessary to distinguish. The solution for t will be a^e times $t(x/b^e)$ plus x^c times a geometric series $\sum_{i=0}^{e-1}\left(\frac{a}{b^c}\right)^i$. The solution for T will be a^e times d plus n^c times a geometric series $\sum_{i=0}^{e-1}\left(\frac{a}{b^c}\right)^i$. In both cases $t(x/b^e)$ (or $T(n/b^e)$) will be d. In both cases the geometric series will be $\Theta(1)$, $\Theta(e)$ or $\Theta\left(\frac{a}{b^c}\right)^e$, depending on whether $\frac{a}{b^c}$ is less than 1, equal to 1, or greater than one. Clearly $e(n) = \log_b n$. Since we must divide x by b an integer number greater than $\log_b x - 1$ times in order to get a value in the range from 1 to b, $e(x) = \lfloor \log_b x \rfloor$. Thus, if m is the largest integer power of b less than or equal to x, then $0 \le e(x) - e(m) < 1$. Let us use r to stand for the real number $\frac{a}{b^c}$. Then we have $r^0 \le r^{e(x)-e(m)} < r$, or $r^{e(m)} \le r^{e(x)} \le r \cdot r^{e(m)}$. Thus we have $r^{e(x)} = \Theta(r^{e(m)})$ Finally, $m^c \le x^c \le b^c m^c$, and so $x^c = \Theta(m^c)$. Therefore, every term of $t(x)$ is Θ of the corresponding term of $T(m)$. Further, there are only a fixed number of different constants involved in our Big-Θ bounds. Therefore since $t(x)$ is composed of sums and products of these terms, $t(x) = \Theta(T(m))$. ■

Theorem 4.13 *Let a and b be positive real numbers with $b \ge 2$ and let c and d be real numbers. Let $T(n)$ be the function defined on the integers by the recurrence*

$$T(n) = \begin{cases} aT(\lceil n/b \rceil) + n^c & \text{if } n \ge b \\ d & n = 1, \end{cases}$$

and let $t(x)$ be the function on the real numbers defined by the recurrence

$$t(x) = \begin{cases} at(x/b) + x^c & \text{if } x \ge b \\ d & \text{if } 1 \le x < b. \end{cases}$$

Then $T(n) = \Theta(t(n))$.

Proof: As in the previous proof, we can iterate both recurrences. Let us compare what the results will be of iterating the recurrence for $t(n)$ and the recurrence for $T(n)$ the same number of times. Note that

$$\begin{aligned} \lceil n/b \rceil &< n/b + 1 \\ \lceil \lceil n/b \rceil / b \rceil < \lceil n/b^2 + 1/b \rceil &< n/b^2 + 1/b + 1 \\ \lceil \lceil \lceil n/b \rceil / b \rceil / b \rceil < \lceil n/b^3 + 1/b^2 + 1/b \rceil &< n/b^3 + 1/b^2 + 1/b + 1 \end{aligned}$$

This suggests that if we define $n_0 = n$, and $n_i = \lceil n_{i-1}/b \rceil$, then, using the fact that $b \ge 2$, it is straightforward to prove by induction, or with the formula for the sum of a geometric series, that $n_i < n/b^i + 2$. The number n_i is the argument of T in the ith iteration of the recurrence for T. We have just seen that it differs from the argument of t in the ith iteration of t by at most 2. In particular, we might have to iterate the recurrence for T twice more than we iterate the recurrence for t to reach the base case. When we iterate the recurrence for t, we get the same solution we got in the previous theorem, with n substituted for x. When we iterate the recurrence for T, we get for some integer j that

$$T(n) = a^j d + \sum_{i=0}^{j-1} a^i n_i^c,$$

with $\frac{n}{b^i} \le n_i \le \frac{n}{b^i} + 2$. But, so long as $n/b^i \ge 2$, we have $n/b^i + 2 \le n/b^{i-1}$. Since the number of iterations of T is at most two more than the number of iterations of t, and since the number of iterations of t is $\lfloor \log_b n \rfloor$, we have that j is at most $\lfloor \log_b n \rfloor + 2$. Therefore all but perhaps the last three values of n_i are less than or equal to n/b^{i-1}, and these last three values are at most b^2, b, and 1. Putting all these bounds together and using $n_0 = n$ gives us

$$\begin{aligned}\sum_{i=0}^{j-1} a^i \left(\frac{n}{b^i}\right)^c &\le \sum_{i=0}^{j-1} a^i n_i^c \\ &\le n^c + \sum_{i=1}^{j-4} a^i \left(\frac{n}{b^{i-1}}\right)^c + a^{j-2}(b^2)^c + a^{j-1}b^c + a^j 1^c,\end{aligned}$$

or

$$\begin{aligned}\sum_{i=0}^{j-1} a^i \left(\frac{n}{b^i}\right)^c &\le \sum_{i=0}^{j-1} a^i n_i^c \\ &\le n^c + b\sum_{i=1}^{j-4} a^i \left(\frac{n}{b^i}\right)^c + a^{j-2}\left(\frac{b^j}{b^{j-2}}\right)^c + a^{j-1}\left(\frac{b^j}{b^{j-1}}\right)^c + a^j\left(\frac{b^j}{b^j}\right)^c.\end{aligned}$$

As we shall see momentarily these last three "extra" terms and the b in front of the summation sign do not change the Big-Θ behavior of the right-hand side.

As in the proof of the master theorem, the Big-Θ behavior of the left hand side depends on whether a/b^c is less than 1, in which case it is $\Theta(n^c)$, equal to 1, in which case it is $\Theta(n^c \log_b n)$, or greater than one in which case it is $\Theta(n^{\log_b a})$. But this is exactly the Big-Θ behavior of the right-hand side, because $n < b^j < nb^2$, so $b^j = \Theta(n)$, which means that $\left(\frac{b^j}{b^i}\right)^c = \Theta\left(\left(\frac{n}{b^i}\right)^c\right)$, and the b in front of the summation sign does not change its Big-Θ behavior. Adding $a^j d$ to the middle term of the inequality to get $T(n)$ does not change this behavior. But this modified middle term is exactly $T(n)$. Since the left and right hand sides have the same big-Θ behavior as $t(n)$, we have T(n) = $\Theta(t(n))$. ■

Important Concepts, Formulas, and Theorems

1. *Master Theorem, simplified version.* The simplified version of the *Master Theorem* states: Let a be an integer greater than or equal to 1 and b be a real number greater than 1. Let c be a positive real number and d a nonnegative real number. Given a recurrence of the form

$$T(n) = \begin{cases} aT(n/b) + n^c & \text{if } n > 1 \\ d & \text{if } n = 1 \end{cases}$$

then for n a power of b,

(a) if $\log_b a < c$, $T(n) = \Theta(n^c)$,

(b) if $\log_b a = c$, $T(n) = \Theta(n^c \log n)$,

(c) if $\log_b a > c$, $T(n) = \Theta(n^{\log_b a})$.

2. *Properties of Logarithms.* For any x, y and z, each greater than 1, $x^{\log_y z} = z^{\log_y x}$. Also, $\log_x y = \Theta(\log_2 y)$.

3. *Master Theorem, More General Version.* Let a and b be positive real numbers with $a \geq 1$ and $b \geq 2$. Let $T(n)$ be defined for powers n of b by

$$T(n) = \begin{cases} aT(n/b) + f(n) & \text{if } n > 1 \\ d & \text{if } n = 1 \end{cases}$$

Then

(a) if $f(n) = \Theta(n^c)$ where $\log_b a < c$, then $T(n) = \Theta(n^c) = \Theta(f(n))$.

(b) if $f(n) = \Theta(n^c)$, where $\log_b a = c$, then $T(n) = \Theta(n^{\log_b a} \log_b n)$

(c) if $f(n) = \Theta(n^c)$, where $\log_b a > c$, then $T(n) = \Theta(n^{\log_b a})$.

A similar result with a base case that depends on b holds when $1 < b < 2$.

4. *Important Recurrences have Unique Solutions. (Optional.)* The recurrence

$$T(n) = \begin{cases} f(n)T(\lceil n/b \rceil) + g(n) & \text{if } n > 1 \\ k & \text{if } n = 1 \end{cases}$$

has a unique solution when f and g are (known) functions defined on the positive integers, and k and b are (known) constants with b an integer larger than 2.

5. *Recurrences Defined on the Positive Real Numbers and Recurrences Defined on the Positive Integers. (Optional.)* Let a and b be positive real numbers with $b > 1$ and c and d be real numbers. Let $t(x)$ be the solution to the recurrence

$$t(x) = \begin{cases} at(x/b) + x^c & \text{if } x \geq b \\ d & \text{if } 1 \leq x < b. \end{cases}$$

Let $T(n)$ be the solution to the recurrence

$$T(n) = \begin{cases} aT(n/b) + n^c & \text{if } n \geq 0 \\ d & \text{if } n = 1, \end{cases}$$

where n is a nonnegative integer power of b. Let $m(x)$ be the largest integer power of b less than or equal to x. Then $t(x) = \Theta(T(m(x)))$

6. *Removing Floors and Ceilings from Recurrences. (Optional.)* Let a and b be positive real numbers with $b \geq 2$ and let c and d be real numbers. Let $T(n)$ be the function defined on the integers by the recurrence

$$T(n) = \begin{cases} aT(\lceil n/b \rceil) + n^c & \text{if } n > 1 \\ d & n = 1 \end{cases},$$

and let $t(x)$ be the function on the real numbers defined by the recurrence

$$t(x) = \begin{cases} at(x/b) + x^c & \text{if } x \geq b \\ d & \text{if } 1 \leq x < b \end{cases}.$$

Then $T(n) = \Theta(t(n))$. The same statement applies with ceilings replaced by floors.

7. *Extending 5 and 6 (Optional.)* In the theorems summarized in 5 and 6 the n^c or x^c term may be replaced by a function f with $f(x) = \Theta(x^c)$.

8. *Solutions to Realistic Recurrences.* The theorems summarized in 5, 6, and 7 tell us that the Big-Θ behavior of solutions to our more realistic recurrences

$$T(n) = \begin{cases} aT(\lceil n/b \rceil) + f(n) & \text{if } n > 1 \\ d & \text{n=1}, \end{cases}$$

where $f(n) = \Theta(n^c)$, is determined by their Big-Θ behavior on powers of the base b and with $f(n) = n^c$.

Problems

1. Use the master theorem to give Big-Θ bounds on the solutions to the following recurrences. For all of these, assume that $T(1) = 1$ and n is a power of the appropriate integer.

   (a) $T(n) = 8T(n/2) + n$

   (b) $T(n) = 8T(n/2) + n^3$

   (c) $T(n) = 3T(n/2) + n$

   (d) $T(n) = T(n/4) + 1$

   (e) $T(n) = 3T(n/3) + n^2$

2. Extend the proof of the Master Theorem, Theorem 4.9 to the case $T(1) = d$.

3. Show that for any x, y and z, each greater than 1, $x^{\log_y z} = z^{\log_y x}$.

4. (Optional) Show that for each real number $x \geq 0$ there is one and only one value of $t(x)$ given by the recurrence

$$t(x) = \begin{cases} 7xt(x-1) + 1 & \text{if } x \geq 1 \\ 1 & \text{if } 0 \leq x < 1. \end{cases}$$

5. (Optional) Show that for each real number $x \geq 1$ there is one and only one value of $t(x)$ given by the recurrence

$$t(x) = \begin{cases} 3xT(x/2) + x^2 & \text{if } x \geq 2 \\ 1 & \text{if } 1 \leq x < 2 \end{cases}.$$

6. (Optional) How many solutions are there to the recurrence

$$T(n) = \begin{cases} f(n)T(\lceil n/b \rceil) + g(n) & \text{if } n > 1 \\ k & \text{if } n = 1 \end{cases}$$

if $b < 2$? If $b = 10/9$, by what would we have to replace the condition that $T(n) = k$ if $n = 1$ in order to get a unique solution?

7. Give a big-Θ bound on the solution to the recurrence

$$T(n) = \begin{cases} 3T(\lceil n/2 \rceil) + \sqrt{n+3} & \text{if } n > 1 \\ d & \text{if } n = 1. \end{cases}$$

8. Give a big-Θ bound on the solution to the recurrence

$$T(n) = \begin{cases} 3T(\lceil n/2 \rceil) + \sqrt{n^3+3} & \text{if } n > 1 \\ d & \text{if } n = 1. \end{cases}$$

9. Give a big-Θ bound on the solution to the recurrence

$$T(n) = \begin{cases} 3T(\lceil n/2 \rceil) + \sqrt{n^4+3} & \text{if } n > 1 \\ d & \text{if } n = 1. \end{cases}$$

10. Give a big-Θ bound on the solution to the recurrence

$$T(n) = \begin{cases} 2T(\lceil n/2 \rceil) + \sqrt{n^2+3} & \text{if } n > 1 \\ d & \text{if } n = 1. \end{cases}$$

11. (Optional) Explain why theorem 4.11 is a consequence of Theorem 4.12 and Theorem 4.13

4.5 More general kinds of recurrences

Recurrence Inequalities

The recurrences we have been working with are really idealized versions of what we know about the problems we are working on. For example, in merge-sort on a list of n items, we say we divide the list into two parts of equal size, sort each part, and then merge the two sorted parts. The time it takes to do this is the time it takes to divide the list into two parts plus the time it takes to sort each part, plus the time it takes to merge the two sorted lists. We don't specify how we are dividing the list, or how we are doing the merging. (We assume the sorting is done by applying the same method to the smaller lists, unless they have size 1, in which case we do nothing.) What we do know is that any sensible way of dividing the list into two parts takes no more than some constant multiple of n time units (and might take no more than constant time if we do it by leaving the list in place and manipulating pointers) and that any sensible algorithm for merging two lists will take no more than some (other) constant multiple of n time units. Thus we know that if $T(n)$ is the amount of time it takes to apply merge sort to n data items, then there is a constant c (the sum of the two constant multiples we mentioned) such that

$$T(n) \leq 2T(n/2) + cn. \tag{4.27}$$

Thus real world problems often lead us to *recurrence inequalities* rather than recurrence equations. These are inequalities that state that $T(n)$ is less than or equal to some expression involving values of $T(m)$ for $m < n$. (We could also include inequalities with a greater than or equal to sign, but they do not arise in the applications we are studying.) A *solution* to a recurrence inequality is a function T that satisfies the inequality. For simplicity we will expand what we mean by the word recurrence to include either recurrence inequalities or recurrence equations.

In Recurrence 4.27 we are implicitly assuming that T is defined only on positive integer values and, since we said we divided the list into two equal parts each time, our analysis only makes sense if we assume that n is a power of 2.

Note that there are actually infinitely many solutions to Recurrence 4.27. (For example for any $c' < c$, the unique solution to

$$T(n) = \begin{cases} 2T(n/2) + c'n & \text{if } n \geq 2 \\ k & \text{if } n = 1 \end{cases} \tag{4.28}$$

satisfies Inequality 4.27 for any constant k.) The idea that Recurrence 4.27 has infinitely many solutions, while Recurrence 4.28 has exactly one solution is analogous to the idea that $x - 3 \leq 0$ has infinitely many solutions while $x - 3 = 0$ has one solution. Later in this section we shall see how to show that all the solutions to Recurrence 4.27 satisfy $T(n) = O(n \log_2 n)$. In other words, no matter how we sensibly implement merge sort, we have a $O(n \log_2 n)$ time bound on how long the merge sort process takes.

Exercise 4.5-1 Carefully prove by induction that for any function T defined on the non-negative powers of 2, if

$$T(n) \leq 2T(n/2) + cn$$

for some constant c, then $T(n) = O(n \log n)$.

A Wrinkle with Induction

We can analyze recurrence inequalities via a recursion tree. The process is virtually identical to our previous use of recursion trees. We must, however, keep in mind that on each level, we are really computing an upper bound on the work done on that level. We can also use a variant of the method we used a few sections ago, guessing an upper bound and verifying by induction. We use this method for the recurrence in Exercise 4.5-1. Here we wish to show that $T(n) = O(n \log n)$. From the definition of Big-O, we can see that we wish to show that $T(n) \leq kn \log n$ for some positive constant k (so long as n is larger than some value n_0).

We are going to do something you may find rather curious. We will consider the possibility that we have a value of k for which the inequality holds. Then in analyzing the consequences of this possibility, we will discover that there are assumptions that we need to make about k in order for such a k to exist. What we will really be doing is experimenting to see how we will need to choose k to make an inductive proof work.

We are given that $T(n) \leq 2T(n/2) + cn$ for all positive integers n that are powers of 2. We want to prove there is another positive real number $k > 0$ and an $n_0 > 0$ such that for $n > n_0$, $T(n) \leq kn \log n$. We cannot expect to have the inequality $T(n) \leq kn \log n$ hold for $n = 1$, because $\log 1 = 0$. To have $T(2) \leq k \cdot 2 \log 2 = k \cdot 2$, we must choose $k \geq \frac{T(2)}{2}$. This is the first assumption we must make about k. Our inductive hypothesis will be that if n is a power of 2 and m is a power of 2 with $2 \leq m < n$ then $T(m) \leq km \log m$. Now $n/2 < n$, and since n is a power of 2 greater than 2, we have that $n/2 \geq 2$, so $(n/2) \log n/2 \geq 2$. By the inductive hypothesis, $T(n/2) \leq k(n/2) \log n/2$. But then

$$\begin{aligned}
T(n) \leq 2T(n/2) + cn &\leq 2k\frac{n}{2}\log\frac{n}{2} + cn && (4.29)\\
&= kn\log\frac{n}{2} + cn && (4.30)\\
&= kn\log n - kn\log 2 + cn && (4.31)\\
&= kn\log n - kn + cn. && (4.32)
\end{aligned}$$

Recall that we are trying to show that $T(n) \leq kn \log n$. But that is not quite what Line 4.32 tells us. This shows that we need to make another assumption about k, namely that $-kn+cn \leq 0$, or $k \geq c$. Then if both our assumptions about k are satisfied, we will have $T(n) < kn \log n$, and we can conclude by the principle of mathematical induction that for all $n > 1$ (so our n_0 is 2), $T(n) \leq kn \log n$, so that $T(n) = O(n \log n)$.

A full inductive proof that $T(n) = O(n \log n)$ is actually embedded in the discussion above, but since it might not appear to everyone to be a proof, below we will summarize our observations in a more traditional looking proof. However you should be aware that some authors and teachers prefer to write their proofs in a style that shows why we make the choices about k that we do, and so you should learn how to to read discussions like the one above as proofs.

We want to show that if $T(n) \leq T(n/2) + cn$, then $T(n) = O(n \log n)$. We are given a real number $c > 0$ such that $T(n) \leq 2T(n/2) + cn$ for all $n > 1$. Choose k to be larger than or equal to $\frac{T(2)}{2}$ and larger than or equal to c. Then

$$T(2) \leq k \cdot 2 \log 2$$

because $k \geq T(n_0)/2$ and $\log 2 = 1$. Now assume that $n > 2$ and assume that for m with $2 \leq m < n$, we have $T(m) \leq km \log m$. Since n is a power of 2, we have $n \geq 4$, so that $n/2$ is an m with $2 \leq m < n$. Thus, by the inductive hypothesis,

$$T\left(\frac{n}{2}\right) \leq k\frac{n}{2}\log\frac{n}{2}.$$

Then by the recurrence,

$$\begin{aligned} T(n) &\leq 2k\frac{n}{2}\log\frac{n}{2} + cn \\ &= kn(\log n - 1) + cn \\ &= kn\log n + cn - kn \\ &\leq kn\log n, \end{aligned}$$

since $k \geq c$. Thus by the principle of mathematical induction, $T(n) \leq kn \log n$ for all $n > 2$, and therefore $T(n) = O(n \log n)$.

There are three things to note about this proof. First without the preceding discussion, the choice of k seems arbitrary. Second, without the preceding discussion, the implicit choice of 2 for the n_0 in the big-O statement also seems arbitrary. Third, the constant k is chosen in terms of the previous constant c. Since c was given to us by the recurrence, it may be used in choosing the constant we use to prove a Big-O statement about solutions to the recurrence. If you compare the formal proof we just gave with the informal discussion that preceded it, you will find each step of the formal proof actually corresponds to something we said in the informal discussion. Since the informal discussion explained why we were making the choices we did, it is natural that some people prefer the informal explanation to the formal proof.

Further Wrinkles in Induction Proofs

Exercise 4.5-2 Suppose that c is a real number greater than zero. Show by induction that any solution $T(n)$ to the recurrence

$$T(n) \leq T(n/3) + cn$$

with n restricted to integer powers of 3 has $T(n) = O(n)$.

Exercise 4.5-3 Suppose that c is a real number greater than zero. Show by induction that any solution $T(n)$ to the recurrence

$$T(n) \leq 4T(n/2) + cn$$

with n restricted to integer powers of 2 has $T(n) = O(n^2)$.

In Exercise 4.5-2 we are given a constant c such that $T(n) \leq T(n/3) + cn$ if $n > 1$. Since we want to show that $T(n) = O(n)$, we want to find two more constants n_0 and k such that $T(n) \leq kn$ whenever $n > n_0$.

We will choose $n_0 = 1$ here. (This was not an arbitrary choice; it is based on observing that $T(1) \leq kn$ is not an impossible condition to satisfy when $n = 1$.) In order to have $T(n) \leq kn$ for

$n = 1$, we must assume $k \geq T(1)$. Now assuming inductively that $T(m) \leq km$ when $1 \leq m < n$ we can write

$$\begin{aligned} T(n) &\leq T(n/3) + cn \\ &\leq k(n/3) + cn \\ &= kn + \left(c - \frac{2k}{3}\right)n \end{aligned}$$

Thus, as long as $c - \frac{2k}{3} \leq 0$, i.e. $k \geq \frac{3}{2}c$, we may conclude by mathematical induction that $T(n) \leq kn$ for all $n \geq 1$. Again, the elements of an inductive proof are in the preceding discussion. Again you should try to learn how to read the argument we just finished as a valid inductive proof. However, we will now present something that looks more like an inductive proof.

We choose k to be the maximum of $T(1)$ and $3c/2$ and we choose $n_0 = 1$. To prove by induction that $T(x) \leq kx$ we begin by observing that $T(1) \leq k \cdot 1$. Next we assume that $n > 1$ and assume inductively that for m with $1 \leq m < n$ we have $T(m) \leq km$. Now we may write

$$T(n) \leq T(n/3) + cn \leq kn/3 + cn = kn + (c - 2k/3)n \leq kn,$$

because we chose k to be at least as large as $3c/2$, making $c - 2k/3$ negative or zero. Thus by the principle of mathematical induction we have $T(n) \leq kn$ for all $n \geq 1$ and so $T(n) = O(n)$.

Now let's analyze Exercise 4.5-3. We won't dot all the i's and cross all the t's here because there is only one major difference between this exercise and the previous one. We wish to prove that there are an n_0 and a k such that $T(n) \leq kn^2$ for $n > n_0$. Assuming that we have chosen n_0 and k so that the base case holds, we can bound $T(n)$ inductively by assuming that $T(m) \leq km^2$ for $m < n$ and reasoning as follows:

$$\begin{aligned} T(n) &\leq 4T\left(\frac{n}{2}\right) + cn \\ &\leq 4\left(k\left(\frac{n}{2}\right)^2\right) + cn \\ &= 4\left(\frac{kn^2}{4}\right) + cn \\ &= kn^2 + cn. \end{aligned}$$

To proceed as before, we would like to choose a value of k so that $cn \leq 0$. But we see that we have a problem because both c and n are always positive! What went wrong? We have a statement that we know is true, and we have a proof method (induction) that worked nicely for similar problems.

The usual way to describe the problem we are facing is that, while the statement is true, it is too weak to be proved by induction. To have a chance of making the inductive proof work, we will have to make an inductive hypothesis that puts some sort of negative quantity, say a term like $-kn$, into the last line of our display above. Let's see if we can prove something that is actually stronger than we were originally trying to prove, namely that for some positive constants k_1 and k_2, $T(n) \leq k_1n^2 - k_2n$. Now proceeding as before, we get

$$T(n) \leq 4T(n/2) + cn$$

$$\begin{aligned}
&\le 4\left(k_1\left(\frac{n}{2}\right)^2 - k_2\left(\frac{n}{2}\right)\right) + cn \\
&= 4\left(\frac{k_1 n^2}{4} - k_2\left(\frac{n}{2}\right)\right) + cn \\
&= k_1 n^2 - 2k_2 n + cn \\
&= k_1 n^2 - k_2 n + (c - k_2)n.
\end{aligned}$$

Now we have to make $(c - k_2)n \le 0$ for the last line to be at most $k_1 n^2 - k_2 n$, and so we just choose $k_2 \ge c$ (and greater than whatever we need in order to make a base case work). Since $T(n) \le k_1 n^2 - k_2 n$ for some constants k_1 and k_2, then $T(n) = O(n^2)$.

At first glance, this approach seems paradoxical: why is it easier to prove a stronger statement than it is to prove a weaker one? This phenomenon happens often in induction: a stronger statement is often easier to prove than a weaker one. Think carefully about an inductive proof where you have assumed that a bound holds for values smaller than n and you are trying to prove a statement for n. You use the bound you have assumed for smaller values to help prove the bound for n. Thus if the bound you used for smaller values is actually weak, then that is hindering you in proving the bound for n. In other words when you want to prove something about $p(n)$ you are using $p(1) \wedge \ldots \wedge p(n-1)$. Thus if these are stronger, they will be of greater help in proving $p(n)$. In the case above, the problem was that the statements, $p(1), \ldots, p(n-1)$ were too weak, and thus we were not able to prove $p(n)$. By using a stronger $p(1), \ldots, p(n-1)$, however, we were able to prove a stronger $p(n)$, one that implied the original $p(n)$ we wanted. When we give an induction proof in this way, we say that we are using a *stronger inductive hypothesis*.

Dealing with Functions Other Than n^c

Our statement of the Master Theorem involved a recursive term plus an added term that was $\Theta(n^c)$. Sometimes algorithmic problems lead us to consider other kinds of functions. The most common such is example is when that added function involves logarithms. For example, consider the recurrence:

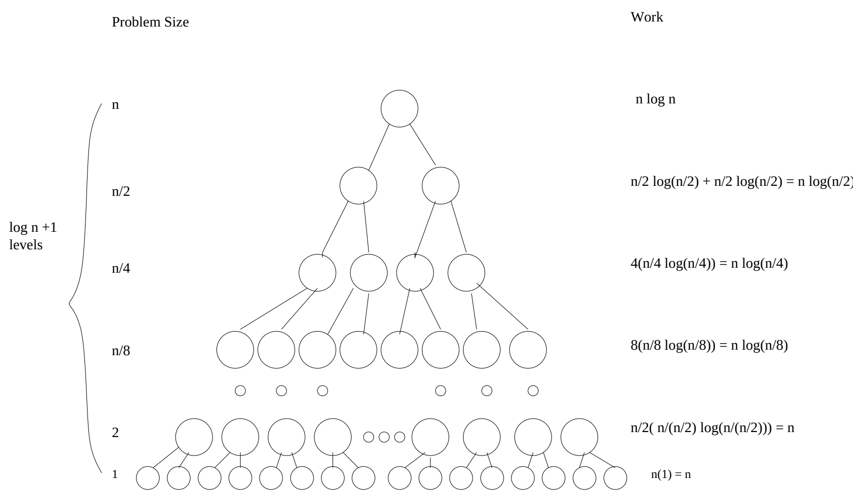
$$T(n) = \begin{cases} 2T(n/2) + n\log n & \text{if } n > 1 \\ 1 & \text{if } n = 1, \end{cases}$$

where n is a power of 2. Just as before, we can draw a recursion tree; the whole methodology works, but our sums may be a little more complicated. The tree for this recurrence is shown in Figure 4.8.

This is similar to the tree for $T(n) = 2T(n/2) + n$, except that the work on level i is $n\log\left(\frac{n}{2^i}\right)$ for $i \ge 2$, and, for the bottom level, it is n, the number of subproblems, times 1. Thus if we sum the work per level we get

$$\begin{aligned}
\sum_{i=0}^{\log n - 1} n\log\left(\frac{n}{2^i}\right) + n &= n\left(\sum_{i=0}^{\log n - 1}\log\left(\frac{n}{2^i}\right) + 1\right) \\
&= n\left(\sum_{i=0}^{\log n - 1}(\log n - \log 2^i) + 1\right)
\end{aligned}$$

Figure 4.8: The recursion tree for $T(n) = 2T(n/2) + n\log n$ if $n > 1$ and $T(1) = 1$.



$$\begin{aligned}
&= n\left(\sum_{i=0}^{\log n-1}\log n - \sum_{i=0}^{\log n-1} i\right) + n \\
&= n\left((\log n)(\log n) - \frac{(\log n)(\log n - 1)}{2}\right) + n \\
&= O(n\log^2 n)\ .
\end{aligned}$$

A bit of mental arithmetic in the second last line of our equations shows that the $\log^2 n$ will not cancel out, so our solution is in fact $\Theta(n\log^2 n)$.

Exercise 4.5-4 Find the best big-O bound you can on the solution to the recurrence

$$T(n) = \begin{cases} T(n/2) + n\log n & \text{if } n > 1 \\ 1 & \text{if } n = 1, \end{cases}$$

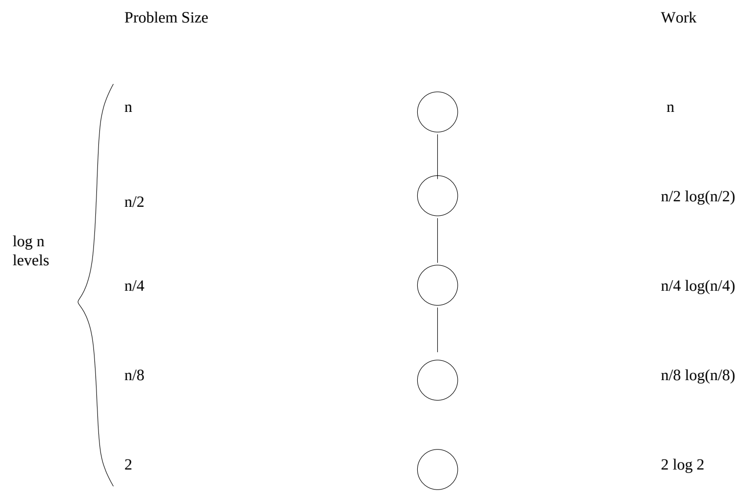
assuming n is a power of 2. Is this bound a big-Θ bound?

The tree for this recurrence is in Figure 4.9

Notice that the work done at the bottom nodes of the tree is determined by the statement $T(1) = 1$ in our recurrence; it is not $1\log 1$. Summing the work, we get

$$\begin{aligned}
1 + \sum_{i=0}^{\log n-1}\frac{n}{2^i}\log\left(\frac{n}{2^i}\right) &= 1 + n\left(\sum_{i=0}^{\log n-1}\frac{1}{2^i}(\log n - \log 2^i)\right) \\
&= 1 + n\left(\sum_{i=0}^{\log n-1}\left(\frac{1}{2}\right)^i(\log(n) - i)\right) \\
&\leq 1 + n\left(\log n \sum_{i=0}^{\log n-1}\left(\frac{1}{2}\right)^i\right)
\end{aligned}$$

Figure 4.9: The recursion tree for the recurrence $T(n) = T(n/2) + n \log n$ if $n > 1$ and $T(1) = 1$.



$$
\begin{aligned}
&\leq 1 + n(\log n)(2) \\
&= O(n \log n).
\end{aligned}
$$

Note that the largest term in the sum in our second line of equations is $\log(n)$, and none of the terms in the sum are negative. This means that n times the sum is at least $n \log n$. Therefore, we have $T(n) = \Theta(n \log n)$.

Removing Ceilings and Using Powers of b. (Optional)

We showed that in our versions of the master theorem, we could ignore ceilings and assume our variables were powers of b. It might appear that the two theorems we used do not apply to the more general functions we have studied in this section any more than the master theorem does. However, they actually only depend on properties of the powers n^c and not the three different kinds of cases, so it turns out we can extend them.

Notice that $(xb)^c = b^c x^c$, and this proportionality holds for all values of x with constant of proportionality b^c. Putting this just a bit less precisely, we can write $(xb)^c = O(x^c)$. This suggests that we might be able to obtain Big-Θ bounds on $T(n)$ when T satisfies a recurrence of the form

$$T(n) = aT(n/b) + f(n)$$

with $f(nb) = \Theta(f(n))$, and we might be able to obtain Big-O bounds on T when T satisfies a recurrence of the form

$$T(n) \leq aT(n/b) + f(n)$$

with $f(nb) = O(f(n))$. But are these conditions satisfied by any functions of practical interest? Yes. For example if $f(x) = \log(x)$, then

$$f(bx) = \log(b) + \log(x) = \Theta(\log(x)).$$

Exercise 4.5-5 Show that if $f(x) = x^2 \log x$, then $f(bx) = \Theta(f(x))$.

Exercise 4.5-6 If $f(x) = 3^x$ and $b = 2$, is $f(bx) = \Theta(f(x))$? Is $f(b(x)) = O(f(x))$?

For Exercise 4.5-5 if $f(x) = x^2 \log x$, then

$$f(bx) = (bx)^2 \log bx = b^2x^2(\log b + \log x) = \Theta(x^2 \log x).$$

However, if $f(x) = 3^x$, then

$$f(2x) = 3^{2x} = (3^x)^2 = 3^x \cdot 3^x,$$

and there is no way that this can be less than or equal to a constant multiple of 3^x, so it is neither $\Theta(3^x)$ nor $O(3^x)$. Our exercises suggest the kinds of functions that satisfy the condition $f(bx) = O(f(x))$ might include at least some of the kinds of functions of x which arise in the study of algorithms. They certainly include the power functions and thus polynomial functions and root functions, or functions bounded by such functions.

There was one other property of power functions n^c that we used implicitly in our discussions of removing floors and ceilings and assuming our variables were powers of b. Namely, if $x > y$ (and $c \geq 0$) then $x^c \geq y^c$. A function f from the real numbers to the real numbers is called *(weakly) increasing* if whenever $x > y$, then $f(x) \geq f(y)$. Functions like $f(x) = \log x$ and $f(x) = x \log x$ are increasing functions. On the other hand, the function defined by

$$f(x) = \begin{cases} x & \text{if } x \text{ is a power of } b \\ x^2 & \text{otherwise} \end{cases}$$

is not increasing even though it does satisfy the condition $f(bx) = \Theta(f(x))$.

Theorem 4.15 *Theorems 4.12 and 4.13 apply to recurrences in which the x^c term is replaced by an increasing function f for which $f(bx) = \Theta(f(x))$.*

Proof: We iterate the recurrences in the same way as in the proofs of the original theorems, and find that the condition $f(bx) = \Theta(f(x))$ applied to an increasing function gives us enough information to again bound the solution to one kind of recurrence above and below with a multiple of the solution of the other kind. The details are similar to those in the original proofs so we omit them. ■

In fact there are versions of Theorems 4.12 and 4.13 for recurrence inequalities also. The proofs involve a similar analysis of iterated recurrences or recursion trees, and so we omit them.

Theorem 4.16 *Let a and b be positive real numbers with $b > 2$ and let $f : R^+ \to R^+$ be an increasing function such that $f(bx) = O(f(x))$. Then every solution $t(x)$ to the recurrence*

$$t(x) \leq \begin{cases} at(x/b) + f(x) & \textit{if } x \geq b \\ c & \textit{if } 1 \leq x < b, \end{cases}$$

where a, b, and c are constants, satisfies $t(x) = O(h(x))$ if and only if every solution $T(n)$ to the recurrence

$$T(n) \leq \begin{cases} aT(n/b) + f(n) & \textit{if } n > 1 \\ d & \textit{if } n = 1, \end{cases}$$

where n is restricted to powers of b, satisfies $T(n) = O(h(n))$.

Theorem 4.17 *Let a and b be positive real numbers with $b \geq 2$ and let $f : R^+ \to R^+$ be an increasing function such that $f(bx) = O(f(x))$. Then every solution $T(n)$ to the recurrence*

$$T(n) \leq \begin{cases} at(\lceil n/b \rceil) + f(n) & \text{if } n > 1 \\ d & \text{if } n = 1, \end{cases}$$

satisfies $T(n) = O(h(n))$ if and only if every solution $t(x)$ to the recurrence

$$t(x) \leq \begin{cases} aT(x/b) + f(x) & \text{if } x \geq b \\ d & \text{if } 1 \leq x < b, \end{cases}$$

satisfies $t(x) = O(h(x))$.

Important Concepts, Formulas, and Theorems

1. *Recurrence Inequality.* Recurrence inequalities are inequalities that state that $T(n)$ is less than or equal to some expression involving values of $T(m)$ for $m < n$. A *solution* to a recurrence inequality is a function T that satisfies the inequality.

2. *Recursion Trees for Recurrence Inequalities.* We can analyze recurrence inequalities via a recursion tree. The process is virtually identical to our previous use of recursion trees. We must, however, keep in mind that on each level, we are really computing an upper bound on the work done on that level.

3. *Discovering Necessary Assumptions for an Inductive Proof.* If we are trying to prove a statement that there is a value k such that an inequality of the form $f(n) \leq kg(n)$ or some other statement that involves the parameter k is true, we may start an inductive proof without knowing a value for k and determine conditions on k by assumptions that we need to make in order for the inductive proof to work. When written properly, such an explanation is actually a valid proof.

4. *Making a Stronger Inductive Hypothesis.* If we are trying to prove by induction a statement of the form $p(n) \Rightarrow q(n)$ and we have a statement $s(n)$ such that $s(n) \Rightarrow q(n)$, it is sometimes useful to try to prove the statement $p(n) \Rightarrow s(n)$. This process is known as proving a *stronger* statement or making a *stronger* inductive hypothesis. It sometimes works because it gives us an inductive hypothesis which suffices to prove the stronger statement even though our original statement $q(n)$ did not give an inductive hypothesis sufficient to prove the original statement. However we must be careful in our choice of $s(n)$, because we have to be able to succeed in proving $p(n) \Rightarrow s(n)$.

5. *When the Master Theorem does not Apply.* To deal with recurrences of the form

   $$T(n) = \begin{cases} aT(\lceil n/b \rceil) + f(n) & \text{if } n > 1 \\ d & \text{if } n = 1 \end{cases}$$

   where $f(n)$ is not $\Theta(n^c)$, recursion trees and iterating the recurrence are appropriate tools even though the Master Theorem does not apply. The same holds for recurrence inequalities.

6. *Increasing function. (Optional.)* A function $f : R \to R$ is said to be *(weakly) increasing* if whenever $x > y$, $f(x) \geq f(y)$

7. *Removing Floors and Ceilings when the Master Theorem does not Apply. (Optional.)* To deal with big-Θ bounds with recurrences of the form

$$T(n) = \begin{cases} aT(\lceil n/b \rceil) + f(n) & \text{if } n > 1 \\ d & \text{if } n = 1 \end{cases}$$

where $f(n)$ is not $\Theta(n^c)$, we may remove floors and ceilings and replace n by powers of b if f is increasing and satisfies the condition $f(nb) = \Theta(f(n))$. To deal with big-O bounds for a similar recurrence inequality we may remove floors and ceilings if f is increasing and satisfies the condition that $f(nb) = O(f(n))$.

Problems

1. (a) Find the best big-O upper bound you can to any solution to the recurrence

$$T(n) = \begin{cases} 4T(n/2) + n \log n & \text{if } n > 1 \\ 1 & \text{if } n = 1. \end{cases}$$

   (b) Assuming that you were able to guess the result you got in part (a), prove by induction that your answer is correct.

2. Is the big-O upper bound in the previous problem actually a big-Θ bound?

3. Show by induction that

$$T(n) = \begin{cases} 8T(n/2) + n \log n & \text{if } n > 1 \\ d & \text{if } n = 1 \end{cases}$$

has $T(n) = O(n^3)$ for any solution $T(n)$.

4. Is the big-O upper bound in the previous problem actually a big-Θ bound?

5. Show by induction that any solution to a recurrence of the form

$$T(n) \leq 2T(n/3) + c \log_3 n$$

is $O(n \log_3 n)$. What happens if you replace 2 by 3 (explain why)? Would it make a difference if we used a different base for the logarithm (only an intuitive explanation is needed here)?

6. What happens if you replace the 2 in Problem 5 by 4? (Hint: one way to attack this is with recursion trees.)

7. Is the big-O upper bound in Problem 5 actually a big Θ bound?

8. (Optional) Give an example (different from any in the text) of a function for which $f(bx) = O(f(x))$. Give an example (different from any in the text) of a function for which $f(bx)$ is not $O(f(x))$.

9. Give the best big O upper bound you can for the solution to the recurrence $T(n) = 2T(n/3 - 3) + n$, and then prove by induction that your upper bound is correct.

10. Find the best big-O upper bound you can to any solution to the recurrence defined on nonnegative integers by
$$T(n) \leq 2T(\lceil n/2 \rceil + 1) + cn.$$
Prove by induction that your answer is correct.

4.6 Recurrences and Selection

The idea of selection

One common problem that arises in algorithms is that of *selection*. In this problem you are given n distinct data items from some set which has an underlying order. That is, given any two items a and b, you can determine whether $a < b$. (Integers satisfy this property, but colors do not.) Given these n items, and some value i, $1 \le i \le n$, you wish to find the ith smallest item in the set. For example in the set

$$\{3, 1, 8, 6, 4, 11, 7\}, \tag{4.33}$$

the first smallest ($i = 1$) is 1, the third smallest ($i = 3$) is 4 and the seventh smallest ($i = n = 7$) is 11. An important special case is that of finding the *median*, which is the case of $i = \lceil n/2 \rceil$. Another important special case is finding percentiles; for example the 90th percentile is the case $i = \lceil .9n \rceil$. As this suggests, i is frequently given as some fraction of n.

Exercise 4.6-1 How do you find the minimum ($i = 1$) or maximum ($i = n$) in a set? What is the running time? How do you find the second smallest element? Does this approach extend to finding the ith smallest? What is the running time?

Exercise 4.6-2 Give the fastest algorithm you can to find the median ($i = \lceil n/2 \rceil$).

In Exercise 4.6-1, the simple $O(n)$ algorithm of going through the list and keeping track of the minimum value seen so far will suffice to find the minimum. Similarly, if we want to find the second smallest, we can go through the list once, find the smallest, remove it and then find the smallest in the new list. This also takes $O(n + n - 1) = O(n)$ time. If we extend this to finding the ith smallest, the algorithm will take $O(in)$ time. Thus for finding the median, this method takes $O(n^2)$ time.

A better idea for finding the median is to first sort the items, and then take the item in position $n/2$. Since we can sort in $O(n \log n)$ time, this algorithm will take $O(n \log n)$ time. Thus if $i = O(\log n)$ we might want to run the algorithm of the previous paragraph, and otherwise run this algorithm.[4]

All these approaches, when applied to the median, take at least some multiple of $(n \log n)$ units of time.[5] The best sorting algorithms take $O(n \log n)$ time also, and one can prove every comparison-based sorting algorithm takes $\Omega(n \log n)$ time. This raises the natural question of whether it is possible to do selection any faster than sorting. In other words, is the problem of finding the median element, or of finding the ith smallest element of a set, significantly easier than the problem of ordering (sorting) the whole set?

A recursive selection algorithm

Suppose for a minute that we magically knew how to find the median in $O(n)$ time. That is, we have a routine MagicMedian, that given as input a set A, returns the median. We could then use this in a divide and conquer algorithm for Select as follows:

[4] We also note that the running time can be improved to $O(n + i \log n)$ by first creating a *heap*, which takes $O(n)$ time, and then performing a Delete-Min operation i times.

[5] An alternate notation for $f(x) = O(g(x))$ is $g(x) = \Omega(f(x))$. Notice the change in roles of f and g. In this notation, we say that all of these algorithms take $\Omega(n \log n)$ time.

```
Select(A, i, n)
(selects the ith smallest element in set A, where n = |A|)
if (n = 1)
      return the one item in A
else
      p = MagicMedian(A)
      Let H be the set of elements greater than p
      Let L be the set of elements less than or equal to p
      if (i ≤ |L|)
            Return Select(L, i, |L|)
      else
            Return Select(H, i − |L|, |H|).
```

By H we do not mean the elements that come after p in the list, but the elements of the list which are larger than p in the underlying ordering of our set. This algorithm is based on the following simple observation. If we could divide the set A up into a "lower half" (L) and an "upper" half (H), then we know in which of these two sets the ith smallest element in A will be. Namely, if $i \le \lceil n/2 \rceil$, it will be in L, and otherwise it will be in H. Thus, we can recursively look in one or the other set. We can easily partition the data into two sets by making two passes, in the first we copy the numbers smaller than p into L, and in the second we copy the numbers larger than p into H.[6]

The only additional detail is that if we look in H, then instead of looking for the ith smallest, we look for the $i - \lceil n/2 \rceil$th smallest, as H is formed by removing the $\lceil n/2 \rceil$ smallest elements from A.

For example, if the input is the set given in 4.33, and p is 6, the set L would be $\{3, 1, 6, 4\}$, and H would be $\{8, 11, 7\}$. If i were 2, we would recurse on the set L, with $i = 2$. On the other hand, if i were 6, we would recurse on the set H, with $i = 6 - 4 = 2$. Observe that the second smallest element in H is 8, as is the sixth smallest element in the original set.

We can express the running time of Select by the following recurrence:

$$T(n) \le T(n/2) + cn \; . \tag{4.34}$$

From the master theorem, we know any function which satisfies this recurrence has $T(n) = O(n)$.

So we can conclude that if we already know how to find the median in linear time, we can design a divide and conquer algorithm that will solve the selection problem in linear time. However, this is nothing to write home about (yet)!

Selection without knowing the median in advance

Sometimes a knowledge of solving recurrences can help us design algorithms. What kinds of recurrences do we know about that have solutions $T(n)$ with $T(n) = O(n)$? In particular, consider recurrences of the form $T(n) \le T(n/b) + cn$, and ask when they have solutions with $T(n) = O(n)$. Using the master theorem, we see that as long as $\log_b 1 < 1$ (and since $\log_b 1 = 0$

[6] We can do this more efficiently, and "in place", using the partition algorithm of quicksort.

for any b, then any b allowed by the master theorem works; that is, any $b > 1$ will work), all solutions to this recurrence will have $T(n) = O(n)$. (Note that b does not have to be an integer.) If we let $b' = 1/b$, we can say equivalently that as long as we can solve a problem of size n by solving (recursively) a problem of size $b'n$, for some $b' < 1$, and also doing $O(n)$ additional work, our algorithm will run in $O(n)$ time. Interpreting this in the selection problem, it says that as long as we can, in $O(n)$ time, choose p to ensure that both L and H have size at most $b'n$, we will have a linear time algorithm. (You might ask "What about actually dividing our set into L and H, doesn't that take some time too?" The answer is yes it does, but we already know we can do the division into H and L in time $O(n)$, so if we can find p in time $O(n)$ also, then we can do both these things in time $O(n)$.)

In particular, suppose that, in $O(n)$ time, we can choose p to ensure that both L and H have size at most $(3/4)n$. Then the running time is described by the recurrence $T(n) = T(3n/4) + O(n)$ and we will be able to solve the selection problem in linear time.

To see why $(3/4)n$ is relevant, suppose instead of the "black box" MagicMedian, we have a much weaker magic black box, one which only guarantees that it will return some number in the middle half of our set in time $O(n)$. That is, it will return a number that is guaranteed to be somewhere between the $n/4$th smallest number and the $3n/4$th smallest number. If we use the number given by this magic box to divide our set into H and L, then neither will have size more than $3n/4$. We will call this black box a MagicMiddle box, and can use it in the following algorithm:

```
Select1(A,i,n)
(selects the ith smallest element in set A, where n = |A| )
if (n = 1)
     return the one item in A
else
     p = MagicMiddle(A)
     Let H be the set of elements greater than p
     Let L be the set of elements less than or equal to p
     if (i ≤ |L|)
          Return Select1(L, i, |L|)
     else
          Return Select1(H, i − |L|, |H|).
```

The algorithm Select1 is similar to Select. The only difference is that p is now only guaranteed to be in the middle half. Now, when we recurse, we decide whether to recruse on L or H based on whether i is less than or equal to $|L|$. The element p is called a *partition element*, because it is used to partition our set A into the two sets L and H.

This is progress, as we now don't need to assume that we can find the median in order to have a linear time algorithm, we only need to assume that we can find one number in the middle half of the set. This problem seems simpler than the original problem, and in fact it is. Thus our knowledge of which recurrences have solutions which are $O(n)$ led us toward a more plausible algorithm.

It takes a clever algorithm to find an item in the middle half of our set. We now describe such an algorithm in which we first choose a subset of the numbers and then *recursively* find the median of that subset.

An algorithm to find an element in the middle half

More precisely, consider the following algorithm in which we assume that $|A|$ is a multiple of 5. (The condition that $n < 60$ in line 2 is a technical condition that will be justified later.)

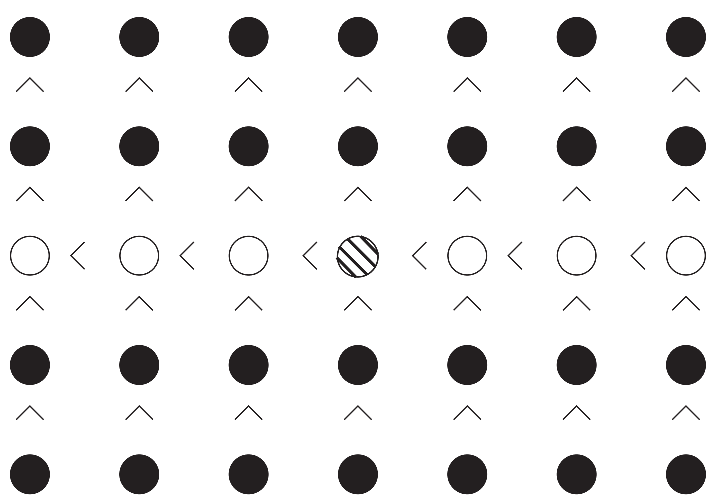
<u>MagicMiddle(A)</u>
(1) Let $n = |A|$
(2) if $(n < 60)$
(3)   use sorting to return the median of A
(4) else
(5)   Break A into $k = n/5$ groups of size 5, $G_1, \ldots, G_k$
(6)   for $i = 1$ to k
(7)   find m_i, the median of G_i (by sorting)
(8)   Let $M = \{m_1, \ldots, m_k\}$
(9)   return Select1 $(M, \lceil k/2 \rceil, k)$.

In this algorithm, we break A into $n/5$ sets of size 5, and then find the median of each set. We then (using Select1 recursively) find the median of medians and return this as our p.

Lemma 4.18 *The value returned by MagicMiddle(A) is in the middle half of A.*

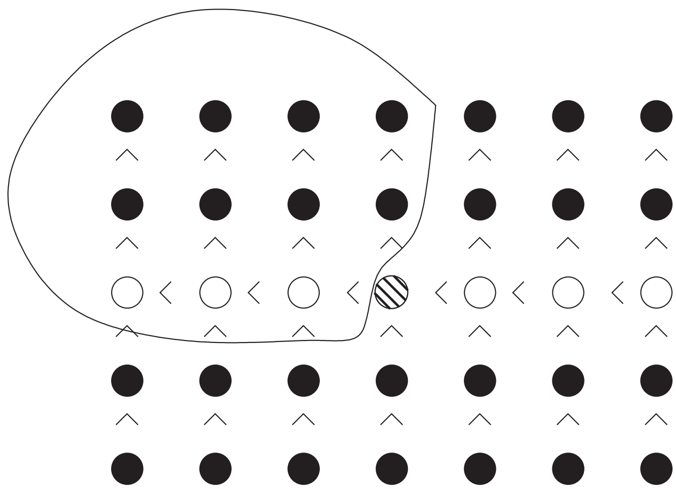
Proof: Consider arranging the elements as follows. List each set of 5 vertically in sorted order, with the smallest element on top. Then line up all $n/5$ of these lists, ordered by their medians, smallest on the left. We get the picture in Figure 4.10. In this picture, the medians

Figure 4.10: Dividing a set into $n/5$ parts of size 5, finding the median of each part and the median of the medians.



are in white, the median of medians is cross-hatched, and we have put in all the inequalities that we know from the ordering information that we have. Now, consider how many items are less than or equal to the median of medians. Every smaller median is clearly less than the median of medians and, in its 5 element set, the elements smaller than the median are also smaller than the median of medians. Now in Figure 4.11 we circle a set of elements that is guaranteed to be smaller than the median of medians. In one fewer (or in the case of an odd number of columns

Figure 4.11: The circled elements are less than the median of the medians.



as in Figure 4.11, one half fewer) than half the columns, we have circled 3 elements and in one column we have circled 2 elements. Therefore, we have circled at least[7]

$$\left(\frac{1}{2}\left(\frac{n}{5}\right) - 1\right)3 + 2 = \frac{3n}{10} - 1$$

elements.

So far we have assumed n is an exact multiple of 5, but we will be using this idea in circumstances when it is not. If it is not an exact multiple of 5, we will have $\lceil n/5 \rceil$ columns (in particular more than $n/5$ columns), but in one of them we might have only one element. It is possible that this column is one of the ones we counted on for 3 elements, so our estimate could be two elements too large.[8] Thus we have circled at least

$$\frac{3n}{10} - 1 - 2 = \frac{3n}{10} - 3$$

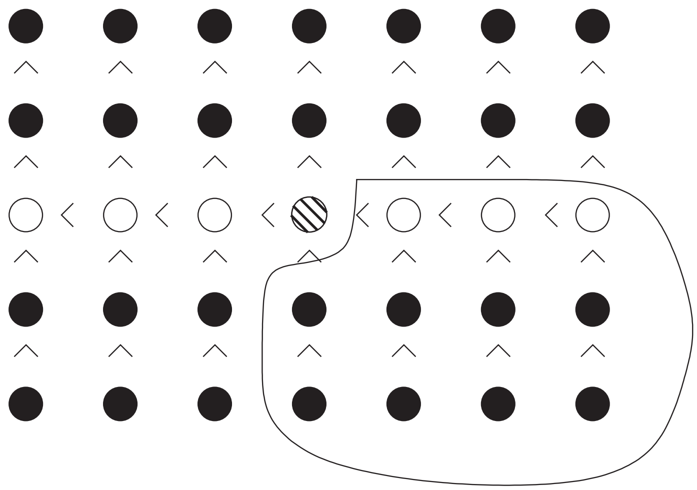
elements. It is a straightforward argument with inequalities that as long as $n \geq 60$, this quantity is at least $n/4$. So if at least $n/4$ items are guaranteed to be less than the median, then at most $3n/4$ items can be greater than the median, and hence $|H| \leq 3n/4$.

A set of elements that is guaranteed to be larger than the median of medians is circled in the Figure 4.12. We can make the same argument about the number of larger elements circled when the number of columns is odd; when the number of columns is even, a similar argument shows that we circle even more elements. By the same argument as we used with $|H|$, this shows that the size of L is at most $3n/4$. ■

[7] We say "at least" because our argument applies exactly when n is even, but underestimates the number of circled elements when n is odd.

[8] A bit less than 2 because we have more than $n/5$ columns.

Figure 4.12: The circled elements are greater than the median of the medians.



Note that we don't actually identify all the nodes that are guaranteed to be, say, less than the median of medians, we are just guaranteed that the proper number exists.

Since we only have the guarantee that MagicMiddle gives us an element in the middle half of the set if the set has at least sixty elements, we modify Select1 to start out by checking to see if $n < 60$, and sorting the set to find the element in position i if $n < 60$. Since 60 is a constant, sorting and finding the desired element takes at most a constant amount of time.

An analysis of the revised selection algorithm

Exercise 4.6-3 Let $T(n)$ be the running time of the modified Select1 on n items. How can you express the running time of Magic Middle in terms of $T(n)$?

Exercise 4.6-4 What is a recurrence for the running time of Select1? Hint: how could Exercise 4.6-3 help you?

Exercise 4.6-5 Can you prove by induction that each solution to the recurrence for Select1 is $O(n)$?

For Exercise 4.6-3, we have the following steps.

- The first step of MagicMiddle is to divide the items into sets of five; this takes $O(n)$ time.
- We then have to find the median of each five-element set. (We can find this median by any straightforward method we choose and still only take at most a constant amount of time; we don't use recursion here.) There are $n/5$ sets and we spend no more than some constant time per set, so the total time is $O(n)$.
- Next we recursively call Select1 to find the median of medians; this takes $T(n/5)$ time.
- Finally, we partition A into those elements less than or equal to the "magic middle" and those that are not, which takes $O(n)$ time.

Thus the total running time is $T(n/5)+O(n)$, which implies that for some n_0 there is a constant $c_0 > 0$ such that, for all $n > n_0$, the running time is no more than $c_0 n$. Even if $n_0 > 60$, there are only finitely many cases between 60 and n_0 so there is a constant c such that for $n \geq 60$, the running time of Magic Middle is no more than $T(n/5) + cn$.

We now get a recurrence for the running time of Select1. Note that for $n \geq 60$ Select1 has to call Magic Middle and then recurse on either L or H, each of which has size at most $3n/4$. For $n < 60$, note that it takes time no more than some constant amount d of time to find the median by sorting. Therefore we get the following recurrence for the running time of Select1:

$$T(n) \leq \begin{cases} T(3n/4) + T(n/5) + c'n & \text{if } n \geq 60 \\ d & \text{if } n < 60. \end{cases} \tag{4.35}$$

This answers Exercise 4.6-4.

As Exercise 4.6-5 requests, we can now verify by induction that $T(n) = O(n)$. What we want to prove is that there is a constant k such that $T(n) \leq kn$. What the recurrence tells us is that there are constants c and d such that $T(n) \leq T(3n/4) + T(n/5) + cn$ if $n \geq 60$, and otherwise $T(n) \leq d$. For the base case we have $T(n) \leq d \leq dn$ for $n < 60$, so we choose k to be at least d and then $T(n) \leq kn$ for $n < 60$. We now assume that $n \geq 60$ and $T(m) \leq km$ for values $m < n$, and get

$$\begin{aligned} T(n) &\leq T(3n/4) + T(n/5) + cn \\ &\leq 3kn/4 + kn/5 + cn \\ &= 19/20kn + cn \\ &= kn + (c - k/20)n \ . \end{aligned}$$

As long as $k \geq 20c$, this is at most kn; so we simply choose k this big and by the principle of mathematical induction, we have $T(n) < kn$ for all positive integers n.

Uneven Divisions

The kind of recurrence we found for the running time of Select1 is actually an instance of a more general class which we will now explore.

Exercise 4.6-6 We already know that when $g(n) = O(n)$, then every solution of $T(n) = T(n/2) + g(n)$ satisfies $T(n) = O(n)$. Use the master theorem to find a Big-O bound to the solution of $T(n) = T(cn) + g(n)$ for any constant $c < 1$, assuming that $g(n) = O(n)$.

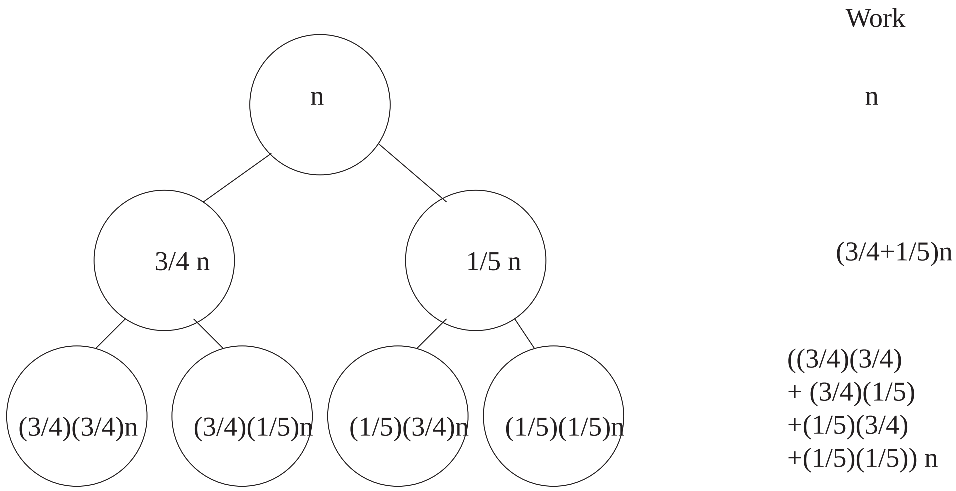
Exercise 4.6-7 Use the master theorem to find Big-O bounds to all solutions of $T(n) = 2T(cn) + g(n)$ for any constant $c < 1/2$, assuming that $g(n) = O(n)$.

Exercise 4.6-8 Suppose $g(n) = O(n)$ and you have a recurrence of the form $T(n) = T(an) + T(bn) + g(n)$ for some constants a and b. What conditions on a and b guarantee that all solutions to this recurrence have $T(n) = O(n)$?

Using the master theorem for Exercise 4.6-6, we get $T(n) = O(n)$, since $\log_{1/c} 1 < 1$. We also get $T(n) = O(n)$ for Exercise 4.6-7, since $\log_{1/c} 2 < 1$ for $c < 1/2$. You might now guess that as long as $a+b<1$, any solution to the recurrence $T(n) \leq T(an)+T(bn)+cn$ has $T(n)=O(n)$. We will now see why this is the case.

First, let's return to the recurrence we had, $T(n) = T(3/4n)+T(n/5)+g(n)$, were $g(n) = O(n)$ and let's try to draw a recursion tree. This recurrence doesn't quite fit our model for recursion trees, as the two subproblems have unequal size (thus we can't even write down the problem size on the left), but we will try to draw a recursion tree anyway and see what happens. As we draw

Figure 4.13: Attempting a recursion tree for $T(n) = T(3/4n) + T(n/5) + g(n)$.



levels one and two, we see that at level one, we have $(3/4 + 1/5)n$ work. At level two we have $((3/4)^2 + 2(3/4)(1/5) + (1/5)^2)n$ work. Were we to work out the third level we would see that we have $((3/4)^3 + 3(3/4)^2(1/5) + 3(3/4)(1/5)^2 + (1/5)^3)n$. Thus we can see a pattern emerging. At level one we have $(3/4+1/5)n$ work. At level 2 we have, by the binomial theorem, $(3/4+1/5)^2 n$ work. At level 3 we have, by the binomial theorem, $(3/4 + 1/5)^3 n$ work. And, similarly, at level i of the tree, we have $\left(\frac{3}{4} + \frac{1}{5}\right)^i n = \left(\frac{19}{20}\right)^i n$ work. Thus summing over all the levels, the total amount of work is

$$\sum_{i=0}^{O(\log n)} \left(\frac{19}{20}\right)^i n \leq \left(\frac{1}{1-19/20}\right) n = 20n.$$

We have actually ignored one detail here. In contrast to a recursion tree in which all subproblems at a level have equal size, the "bottom" of the tree is more complicated. Different branches of the tree will reach problems of size 1 and terminate at different levels. For example, the branch that follows all 3/4's will bottom out after $\log_{4/3} n$ levels, while the one that follows all 1/5's will bottom out after $\log_5 n$ levels. However, the analysis above *overestimates the work*. That is, it assumes that nothing bottoms out until everything bottoms out, i.e. at $\log_{20/19} n$ levels. In fact, the upper bound we gave on the sum "assumes" that the recurrence never bottoms out.

We see here something general happening. It seems as if to understand a recurrence of the form $T(n) = T(an) + T(bn) + g(n)$, with $g(n) = O(n)$, we can study the simpler recurrence $T(n) = T((a+b)n) + g(n)$ instead. This simplifies things (in particular, it lets us use the Master Theorem) and allows us to analyze a larger class of recurrences. Turning to the median algorithm, it tells us that the important thing that happened there was that the sizes of the two recursive calls, namely $3/4n$ and $n/5$, summed to less than 1. As long as that is the case for an algorithm with two recursive calls and an $O(n)$ additional work term, whose recurrence has the form $T(n) = T(an) + T(bn) + g(n)$, with $g(n) = O(n)$, the algorithm will work in $O(n)$ time.

Important Concepts, Formulas, and Theorems

1. *Median.* The *median* of a set (with an underlying order) of n elements is the element that would be in position $\lceil n/2 \rceil$ if the set were sorted into a list in order.

2. *Percentile.* The pth percentile of a set (with an underlying order) is the element that would be in position $\lceil \frac{p}{100} n \rceil$ if the set were sorted into a list in order.

3. *Selection.* Given an n-element set with some underlying order, the problem of *selection* of the ith smallest element is that of finding the element that would be in the ith position if the set were sorted into a list in order. Note that often i is expressed as a fraction of n.

4. *Partition Element.* A *partition element* in an algorithm is an element of a set (with an underlying order) which is used to divide the set into two parts, those that come before or are equal to the element (in the underlying order), and the remaining elements. Notice that the set as given to the algorithm is not necessarily (in fact not usually) given in the underlying order.

5. *Linear Time Algorithms.* If the running time of an algorithm satisfies a recurrence of the form $T(n) \leq T(an) + cn$ with $0 \leq a < 1$, or a recurrence of the form $T(n) \leq T(an) + T(bn) + cn$ with a and b nonnegative and $a + b < 1$, then $T(n) = O(n)$.

6. *Finding a Good Partition Element.* If a set (with an underlying order) has sixty or more elements, then the procedure of breaking the set into pieces of size 5 (plus one leftover piece if necessary), finding the median of each piece and then finding the median of the medians gives an element guaranteed to be in the middle half of the set.

7. *Selection algorithm.* The Selection algorithm that runs in linear time sorts a set of size less than sixty to find the element in the ith position; otherwise

   - it recursively uses the median of medians of five to find a partition element,
   - it uses that partition element to divide the set into two pieces and
   - then it looks for the appropriate element in the appropriate piece recursively.

Problems

1. In the MagicMiddle algorithm, suppose we broke our data up into $n/3$ sets of size 3. What would the running time of Select1 be?

2. In the MagicMiddle algorithm, suppose we broke our data up into $n/7$ sets of size 7. What would the running time of Select1 be?

3. Let

$$T(n) = \begin{cases} T(n/3) + T(n/2) + n & \text{if } n \geq 6 \\ 1 & \text{otherwise,} \end{cases}$$

and let

$$S(n) = \begin{cases} S(5n/6) + n & \text{if } n \geq 6 \\ 1 & \text{otherwise.} \end{cases}$$

Draw recursion trees for T and S. What are the big-O bounds we get on solutions to the recurrences? Use the recursion trees to argue that, for all n, $T(n) \leq S(n)$.

4. Find a (big-O) upper bound (the best you know how to get) on solutions to the recurrence $T(n) = T(n/3) + T(n/6) + T(n/4) + n$.

5. Find a (big-O) upper bound (the best you know how to get) on solutions the recurrence $T(n) = T(n/4) + T(n/2) + n^2$.

6. Note that we have chosen the median of an n-element set to be the element in position $\lceil n/2 \rceil$. We have also chosen to put the median of the medians into the set L of algorithm Select1. Show that this lets us prove that $T(n) \leq T(3n/4) + T(n/5) + cn$ for $n \geq 40$ rather than $n \geq 60$. (You will need to analyze the case where $\lceil n/5 \rceil$ is even and the case where it is odd separately.) Is 40 the least value possible?

Chapter 5

Probability

5.1 Introduction to Probability

Why do we study probability?

You have likely studied hashing as a way to store data (or keys to find data) in a way that makes it possible to access that data quickly. Recall that we have a table in which we want to store keys, and we compute a function h of our key to tell us which location (also known as a "slot" or a "bucket") in the table to use for the key. Such a function is chosen with the hope that it will tell us to put different keys in different places, but with the realization that it might not. If the function tells us to put two keys in the same place, we might put them into a linked list that starts at the appropriate place in the table, or we might have some strategy for putting them into some other place in the table itself. If we have a table with a hundred places and fifty keys to put in those places, there is no reason in advance why all fifty of those keys couldn't be assigned (hashed) to the same place in the table. However someone who is experienced with using hash functions and looking at the results will tell you you'd never see this in a million years. On the other hand that same person would also tell you that you'd never see all the keys hash into different locations in a million years either. In fact, it is far less likely that all fifty keys would hash into one place than that all fifty keys would hash into different places, but both events are quite unlikely. Being able to understand just how likely or unlikely such events are is our reason for taking up the study of probability.

In order to assign probabilities to events, we need to have a clear picture of what these events are. Thus we present a model of the kinds of situations in which it is reasonable to assign probabilities, and then recast our questions about probabilities into questions about this model. We use the phrase *sample space* to refer to the set of possible outcomes of a process. For now, we will deal with processes that have finite sample spaces. The process might be a game of cards, a sequence of hashes into a hash table, a sequence of tests on a number to see if it fails to be a prime, a roll of a die, a series of coin flips, a laboratory experiment, a survey, or any of many other possibilities. A set of elements in a sample space is called an *event*. For example, if a professor starts each class with a 3 question true-false quiz the sample space of all possible patterns of correct answers is

$$\{TTT, TTF, TFT, FTT, TFF, FTF, FFT, FFF\}.$$

The event of the first two answers being true is $\{TTT, TTF\}$. In order to compute probabilities we assign a *probability weight* $p(x)$ to each element of the sample space so that the weight represents what we believe to be the relative likelihood of that outcome. There are two rules we must follow in assigning weights. First the weights must be nonnegative numbers, and second the sum of the weights of all the elements in a sample space must be one. We define the *probability* $P(E)$ of the event E to be the sum of the weights of the elements of E. Algebraically we can write

$$P(E) = \sum_{x:x\in E} p(x). \tag{5.1}$$

We read this as $p(E)$ equals the sum, over all x such that x is in E, of $p(x)$.

Notice that a probability function P on a sample space S satisfies the rules[1]

1. $P(A) \geq 0$ for any $A \subseteq S$.
2. $P(S) = 1$.
3. $P(A \cup B) = P(A) + P(B)$ for any two disjoint events A and B.

The first two rules reflect our rules for assigning weights above. We say that two events are disjoint if $A \cap B = \emptyset$. The third rule follows directly from the definition of disjoint and our definition of the probability of an event. A function P satisfying these rules is called a *probability distribution* or a *probability measure*.

In the case of the professor's three question quiz, it is natural to expect each sequence of trues and falses to be equally likely. (A professor who showed any pattern of preferences would end up rewarding a student who observed this pattern and used it in educated guessing.) Thus it is natural to assign equal weight 1/8 to each of the eight elements of our quiz sample space. Then the *probability* of an event E, which we denote by $P(E)$, is the sum of the weights of its elements. Thus the probability of the event "the first answer is T" is $\frac{1}{8}+\frac{1}{8}+\frac{1}{8}+\frac{1}{8}=\frac{1}{2}$. The event "There is at exactly one True" is $\{TFF, FTF, FFT\}$, so $P(\text{there is exactly one True})$ is 3/8.

Some examples of probability computations

Exercise 5.1-1 Try flipping a coin five times. Did you get at least one head? Repeat five coin flips a few more times! What is the probability of getting at least one head in five flips of a coin? What is the probability of no heads?

Exercise 5.1-2 Find a good sample space for rolling two dice. What weights are appropriate for the members of your sample space? What is the probability of getting a 6 or 7 total on the two dice? Assume the dice are of different colors. What is the probability of getting less than 3 on the red one and more than 3 on the green one?

Exercise 5.1-3 Suppose you hash a list of n keys into a hash table with 20 locations. What is an appropriate sample space, and what is an appropriate weight function? (Assume the keys and the hash function are not in any special relationship to the

[1] These rules are often called "the axioms of probability." For a finite sample space, we could show that if we started with these axioms, our definition of probability in terms of the weights of individual elements of S is the only definition possible. That is, for any other definition, the probabilities we would compute would still be the same if we take $w(x) = P(\{x\})$.

number 20.) If n is three, what is the probability that all three keys hash to different locations? If you hash ten keys into the table, what is the probability that at least two keys have hashed to the same location? We say two keys *collide* if they hash to the same location. How big does n have to be to insure that the probability is at least one half that has been at least one collision?

In Exercise 5.1-1 a good sample space is the set of all 5-tuples of Hs and Ts. There are 32 elements in the sample space, and no element has any reason to be more likely than any other, so a natural weight to use is $\frac{1}{32}$ for each element of the sample space. Then the event of at least one head is the set of all elements but $TTTTT$. Since there are 31 elements in this set, its probability is $\frac{31}{32}$. This suggests that you should have observed at least one head pretty often!

Complementary probabilities

The probability of no heads is the weight of the set $\{TTTTT\}$, which is $\frac{1}{32}$. Notice that the probabilities of the event of "no heads" and the opposite event of "at least one head" add to one. This observation suggests a theorem. The *complement* of an event E in a sample space S, denoted by $S-E$, is the set of all outcomes in S but not E. The theorem tells us how to compute the probability of the complement of an event from the probability of the event.

Theorem 5.1 *If two events E and F are complementary, that is they have nothing in common ($E \cap F = \emptyset$) and their union is the whole sample space ($E \cup F = S$), then*

$$P(E) = 1 - P(F).$$

Proof: The sum of all the probabilities of all the elements of the sample space is one, and since we can break this sum into the sum of the probabilities of the elements of E plus the sum of the probabilities of the elements of F, we have

$$P(E) + P(F) = 1,$$

which gives us $P(E) = 1 - P(F)$.■

For Exercise 5.1-2 a good sample space would be pairs of numbers (a, b) where $(1 \le a, b \le 6)$. By the product principle[2], the size of this sample space is $6 \cdot 6 = 36$. Thus a natural weight for each ordered pair is $\frac{1}{36}$. How do we compute the probability of getting a sum of six or seven? There are 5 ways to roll a six and 6 ways to roll a seven, so our event has eleven elements each of weight $1/36$. Thus the probability of our event is is $11/36$. For the question about the red and green dice, there are two ways for the red one to turn up less than 3, and three ways for the green one to turn up more than 3. Thus, the event of getting less than 3 on the red one and greater than 3 on the green one is a set of size $2 \cdot 3 = 6$ by the product principle. Since each element of the event has weight $1/36$, the event has probability $6/36$ or $1/6$.

[2]From Section 1.1.

Probability and hashing

In Exercise 5.1-3 an appropriate sample space is the set of n-tuples of numbers between 1 and 20. The first entry in an n-tuple is the position our first key hashes to, the second entry is the position our second key hashes to, and so on. Thus each n tuple represents a possible hash function, and each hash function, applied to our keys, would give us one n-tuple. The size of the sample space is 20^n (why?), so an appropriate weight for an n-tuple is $1/20^n$. To compute the probability of a collision, we will first compute the probability that all keys hash to different locations and then apply Theorem 5.1 which tells us to subtract this probability from 1 to get the probability of collision.

To compute the probability that all keys hash to different locations we consider the event that all keys hash to different locations. This is the set of n tuples in which all the entries are different. (In the terminology of functions, these n-tuples correspond to one-to-one hash functions). There are 20 choices for the first entry of an n-tuple in our event. Since the second entry has to be different, there are 19 choices for the second entry of this n-tuple. Similarly there are 18 choices for the third entry (it has to be different from the first two), 17 for the fourth, and in general $20 - i + 1$ possibilities for the ith entry of the n-tuple. Thus we have

$$20 \cdot 19 \cdot 18 \cdot \dots \cdot (20 - n + 1) = 20^{\underline{n}}$$

elements of our event.[3] Since each element of this event has weight $1/20^n$, the probability that all the keys hash to different locations is

$$\frac{20 \cdot 19 \cdot 18 \cdot \dots \cdot (20 - n + 1)}{20^n} = \frac{20^{\underline{n}}}{20^n.}$$

In particular if n is 3 the probability is $(20 \cdot 19 \cdot 18)/20^3 = .855$.

We show the values of this function for n between 0 and 20 in Table 5.1. Note how quickly the probability of getting a collision grows. As you can see with $n = 10$, the probability that there have been no collisions is about .065, so the probability of at least one collision is .935.

If $n = 5$ this number is about .58, and if $n = 6$ this number is about .43. By Theorem 5.1 the probability of a collision is one minus the probability that all the keys hash to different locations. Thus if we hash six items into our table, the probability of a collision is more than 1/2. Our first intuition might well have been that we would need to hash ten items into our table to have probability 1/2 of a collision. This example shows the importance of supplementing intuition with careful computation!

The technique of computing the probability of an event of interest by first computing the probability of its complementary event and then subtracting from 1 is very useful. You will see many opportunities to use it, perhaps because about half the time it is easier to compute directly the probability that an event doesn't occur than the probability that it does. We stated Theorem 5.1 as a theorem to emphasize the importance of this technique.

The Uniform Probability Distribution

In all three of our exercises it was appropriate to assign the same weight to all members of our sample space. We say P is the *uniform probability measure* or *uniform probability distribution*

[3]Using the notation for falling factorial powers that we introduced in Section 1.2.

n	Prob of empty slot	Prob of no collisions
1	1	1
2	0.95	0.95
3	0.9	0.855
4	0.85	0.72675
5	0.8	0.5814
6	0.75	0.43605
7	0.7	0.305235
8	0.65	0.19840275
9	0.6	0.11904165
10	0.55	0.065472908
11	0.5	0.032736454
12	0.45	0.014731404
13	0.4	0.005892562
14	0.35	0.002062397
15	0.3	0.000618719
16	0.25	0.00015468
17	0.2	3.09359E-05
18	0.15	4.64039E-06
19	0.1	4.64039E-07
20	0.05	2.3202E-08

Table 5.1: The probabilities that all elements of a set hash to different entries of a hash table of size 20.

when we assign the same probability to all members of our sample space. The computations in the exercises suggest another useful theorem.

Theorem 5.2 *Suppose P is the uniform probability measure defined on a sample space S. Then for any event E,*

$$P(E) = |E|/|S|,$$

the size of E divided by the size of S.

Proof: Let $S = \{x_1, x_2, \ldots, x_{|S|}\}$. Since P is the uniform probability measure, there must be some value p such that for each $x_i \in S, P(x_i) = p$. Combining this fact with the second and third probability rules, we obtain

$$\begin{aligned} 1 &= P(S) \\ &= P(x_1 \cup x_2 \cup \cdots \cup x_{|S|}) \\ &= P(x_1) + P(x_2) + \ldots + P(x_{|S|}) \\ &= p|S| \ . \end{aligned}$$

Equivalently

$$p = \frac{1}{|S|} \ . \tag{5.2}$$

E is a subset of S with $|E|$ elements and therefore

$$P(E) = \sum_{x_i \in E} p(x_i) = |E|p \ . \tag{5.3}$$

Combining equations 5.2 and 5.3 gives that $P(E) = |E|p = |E|(1/|S|) = |E|/|S|$. ■

Exercise 5.1-4 What is the probability of an odd number of heads in three tosses of a coin? Use Theorem 5.2.

Using a sample space similar to that of first example (with "T" and "F" replaced by "H" and "T"), we see there are three sequences with one H and there is one sequence with three H's. Thus we have four sequences in the event of "an odd number of heads come up." There are eight sequences in the sample space, so the probability is $\frac{4}{8} = \frac{1}{2}$.

It is comforting that we got one half because of a symmetry inherent in this problem. In flipping coins, heads and tails are equally likely. Further if we are flipping 3 coins, an odd number of heads implies an even number of tails. Therefore, the probability of an odd number of heads, even number of heads, odd number of tails and even number of tails must all be the same. Applying Theorem 5.1 we see that the probability must be 1/2.

A word of caution is appropriate here. Theorem 5.2 applies only to probabilities that come from the equiprobable weighting function. The next example shows that it does not apply in general.

Exercise 5.1-5 A sample space consists of the numbers 0, 1, 2 and 3. We assign weight $\frac{1}{8}$ to 0, $\frac{3}{8}$ to 1, $\frac{3}{8}$ to 2, and $\frac{1}{8}$ to 3. What is the probability that an element of the sample space is positive? Show that this is not the result we would obtain by using the formula of Theorem 5.2.

The event "x is positive" is the set $E = \{1, 2, 3\}$. The probability of E is

$$P(E) = P(1) + P(2) + P(3) = \frac{3}{8} + \frac{3}{8} + \frac{1}{8} = \frac{7}{8} \, .$$

However, $\frac{|E|}{|S|} = \frac{3}{4}$.

The previous exercise may seem to be "cooked up" in an unusual way just to prove a point. In fact that sample space and that probability measure could easily arise in studying something as simple as coin flipping.

Exercise 5.1-6 Use the set $\{0, 1, 2, 3\}$ as a sample space for the process of flipping a coin three times and counting the number of heads. Determine the appropriate probability weights $P(0)$, $P(1)$, $P(2)$, and $P(3)$.

There is one way to get the outcome 0, namely tails on each flip. There are, however, three ways to get 1 head and three ways to get two heads. Thus $P(1)$ and $P(2)$ should each be three times $P(0)$. There is one way to get the outcome 3—heads on each flip. Thus $P(3)$ should equal $P(0)$. In equations this gives $P(1) = 3P(0)$, $P(2) = 3P(0)$, and $P(3) = P(0)$. We also have the equation saying all the weights add to one, $P(0) + P(1) + P(2) + P(3) = 1$. There is one and only one solution to these equations, namely $P(0) = \frac{1}{8}$, $P(1) = \frac{3}{8}$, $P(2) = \frac{3}{8}$, and $P(3) = \frac{1}{8}$. Do you notice a relationship between $P(x)$ and the binomial coefficient $\binom{3}{x}$ here? Can you predict the probabilities of 0, 1, 2, 3, and 4 heads in four flips of a coin?

Together, the last two exercises demonstrate that we must be careful not to apply Theorem 5.2 unless we are using the uniform probability measure.

Important Concepts, Formulas, and Theorems

1. *Sample Space.* We use the phrase *sample space* to refer to the set of possible outcomes of a process.

2. *Event.* A set of elements in a sample space is called an *event*.

3. *Probability.* In order to compute probabilities we assign a *weight* to each element of the sample space so that the weight represents what we believe to be the relative likelihood of that outcome. There are two rules we must follow in assigning weights. First the weights must be nonnegative numbers, and second the sum of the weights of all the elements in a sample space must be one. We define the *probability* $P(E)$ of the event E to be the sum of the weights of the elements of E.

4. *The axioms of Probability.* Three rules that a probability measure on a finite sample space must satisfy could actually be used to define what we mean by probability.

   (a) $P(A) \geq 0$ for any $A \subseteq S$.

   (b) $P(S) = 1$.

   (c) $P(A \cup B) = P(A) + P(B)$ for any two disjoint events A and B.

5. *Probability Distribution.* A function which assigns a probability to each member of a sample space is called a (discrete) *probability distribution*.

6. *Complement.* The *complement* of an event E in a sample space S, denoted by $S - E$, is the set of all outcomes in S but not E.

7. The Probabilities of Complementary Events. If two events E and F are complementary, that is they have nothing in common ($E \cap F = \emptyset$), and their union is the whole sample space ($E \cup F = S$), then
$$P(E) = 1 - P(F).$$

8. *Collision, Collide (in Hashing).* We say two keys *collide* if they hash to the same location.

9. *Uniform Probability Distribution.* We say P is the *uniform probability measure* or *uniform probability distribution* when we assign the same probability to all members of our sample space.

10. *Computing Probabilities with the Uniform Distribution.* Suppose P is the uniform probability measure defined on a sample space S. Then for any event E,
$$P(E) = |E|/|S|,$$
the size of E divided by the size of S. This *does not* apply to general probability distributions.

Problems

1. What is the probability of exactly three heads when you flip a coin five times? What is the probability of three or more heads when you flip a coin five times?

2. When we roll two dice, what is the probability of getting a sum of 4 or less on the tops?

3. If we hash 3 keys into a hash table with ten slots, what is the probability that all three keys hash to different slots? How big does n have to be so that if we hash n keys to a hash table with 10 slots, the probability is at least a half that some slot has at least two keys hash to it? How many keys do we need to have probability at least two thirds that some slot has at least two keys hash to it?

4. What is the probability of an odd sum when we roll three dice?

5. Suppose we use the numbers 2 through 12 as our sample space for rolling two dice and adding the numbers on top. What would we get for the probability of a sum of 2, 3, or 4, if we used the equiprobable measure on this sample space. Would this make sense?

6. Two pennies, a nickel and a dime are placed in a cup and a first coin and a second coin are drawn.

   (a) Assuming we are sampling without replacement (that is, we don't replace the first coin before taking the second) write down the sample space of all ordered pairs of letters P, N, and D that represent the outcomes. What would you say are the appropriate weights for the elements of the sample space?

   (b) What is the probability of getting eleven cents?

7. Why is the probability of five heads in ten flips of a coin equal to $\frac{63}{256}$?

8. Using 5-element sets as a sample space, determine the probability that a "hand" of 5 cards chosen from an ordinary deck of 52 cards will consist of cards of the same suit.

9. Using 5 element permutations as a sample space, determine the probability that a "hand" of 5 cards chosen from an ordinary deck of 52 cards will have all the cards from the same suit

10. How many five-card hands chosen from a standard deck of playing cards consist of five cards in a row (such as the nine of diamonds, the ten of clubs, jack of clubs, queen of hearts, and king of spades)? Such a hand is called a straight. What is the probability that a five-card hand is a straight? Explore whether you get the same answer by using five element sets as your model of hands or five element permutations as your model of hands.

11. A student taking a ten-question, true-false diagnostic test knows none of the answers and must guess at each one. Compute the probability that the student gets a score of 80 or higher. What is the probability that the grade is 70 or lower?

12. A die is made of a cube with a square painted on one side, a circle on two sides, and a triangle on three sides. If the die is rolled twice, what is the probability that the two shapes we see on top are the same?

13. Are the following two events equally likely? Event 1 consists of drawing an ace and a king when you draw two cards from among the thirteen spades in a deck of cards and event 2 consists of drawing an ace and a king when you draw two cards from the whole deck.

14. There is a retired professor who used to love to go into a probability class of thirty or more students and announce "I will give even money odds that there are two people in this classroom with the same birthday." With thirty students in the room, what is the probability that all have different birthdays? What is the minimum number of students that must be in the room so that the professor has at least probability one half of winning the bet? What is the probability that he wins his bet if there are 50 students in the room. Does this probability make sense to you? (There is no wrong answer to that question!) Explain why or why not.

5.2 Unions and Intersections

The probability of a union of events

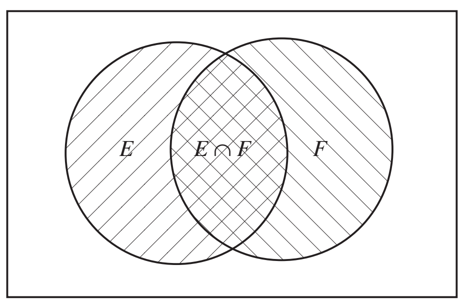
Exercise 5.2-1 If you roll two dice, what is the probability of an even sum or a sum of 8 or more?

Exercise 5.2-2 In Exercise 5.2-1, let E be the event "even sum" and let F be the event "8 or more." We found the probability of the union of the events E and F. Why isn't it the case that $P(E \cup F) = P(E) + P(F)$? What weights appear twice in the sum $P(E) + P(F)$? Find a formula for $P(E \cup F)$ in terms of the probabilities of E, F, and $E \cap F$. Apply this formula to Exercise 5.2-1. What is the value of expressing one probability in terms of three?

Exercise 5.2-3 What is $P(E \cup F \cup G)$ in terms of probabilities of the events E, F, and G and their intersections?

In the sum $P(E) + P(F)$ the weights of elements of $E \cap F$ each appear twice, while the weights of all other elements of $E \cup F$ each appear once. We can see this by looking at a diagram called a Venn Diagram, as in Figure 5.1. In a *Venn diagram*, the rectangle represents the sample space, and the circles represent the events. If we were to shade both E and F, we would wind

Figure 5.1: A Venn diagram for two events.



up shading the region $E \cap F$ twice. In Figure 5.2, we represent that by putting numbers in the regions, representing how many times they are shaded. This illustrates why the sum $P(E)+P(F)$ includes the probability weight of each element of $E \cap F$ twice. Thus to get a sum that includes the probability weight of each element of $E \cup F$ exactly once, we have to subtract the weight of $E \cap F$ from the sum $P(E) + P(F)$. This is why

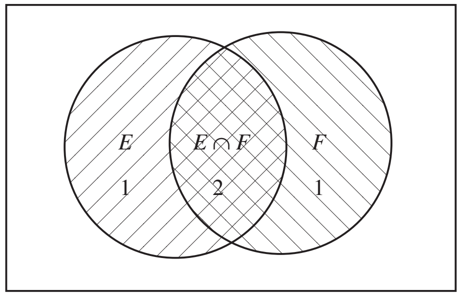
$$P(E \cup F) = P(E) + P(F) - P(E \cap F) \tag{5.4}$$

.

We can now apply this to Exercise 5.2-1 by noting that the probability of an even sum is 1/2, while the probability of a sum of 8 or more is

$$\frac{1}{36} + \frac{2}{36} + \frac{3}{36} + \frac{4}{36} + \frac{5}{36} = \frac{15}{36}.$$

Figure 5.2: If we shade each of E and F once, then we shade $E \cap F$ twice



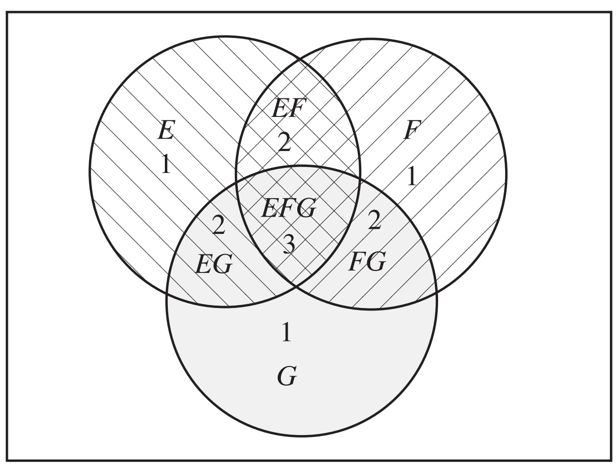
From a similar sum, the probability of an even sum of 8 or more is 9/36, so the probability of a sum that is even or is 8 or more is

$$\frac{1}{2} + \frac{15}{36} - \frac{9}{36} = \frac{2}{3}.$$

(In this case our computation merely illustrates the formula; with less work one could add the probability of an even sum to the probability of a sum of 9 or 11.) In many cases, however, probabilities of individual events and their intersections are more straightforward to compute than probabilities of unions (we will see such examples later in this section), and in such cases our formula is quite useful.

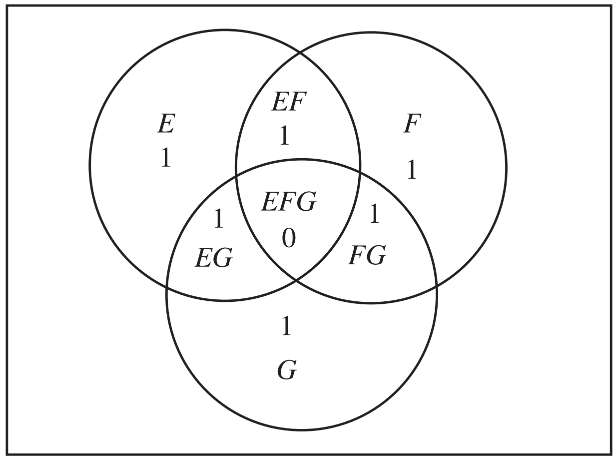
Now let's consider the case for three events and draw a Venn diagram and fill in the numbers for shading all E, F, and G. So as not to crowd the figure we use EF to label the region corresponding to $E \cap F$, and similarly label other regions. Doing so we get Figure 5.3. Thus we

Figure 5.3: The number of ways the intersections are shaded when we shade E, F, and G.



have to figure out a way to subtract from $P(E) + P(F) + P(G)$ the weights of elements in the regions labeled EF, FG and EG once, and the the weight of elements in the region labeled EFG twice. If we subtract out the weights of elements of each of $E \cap F$, $F \cap G$, and $E \cap G$, this does more than we wanted to do, as we subtract the weights of elements in EF, FG and EG once but the weights of elements in of EFG three times, leaving us with Figure 5.4. We then see that

Figure 5.4: The result of removing the weights of each intersection of two sets.



all that is left to do is to add weights of elements in the $E \cap F \cap G$ back into our sum. Thus we have that

$$P(E \cup F \cup G) = P(E) + P(F) + P(G) - P(E \cap F) - P(E \cap G) - P(F \cap G) + P(E \cap F \cap G).$$

Principle of inclusion and exclusion for probability

From the last two exercises, it is natural to guess the formula

$$P(\bigcup_{i=1}^{n} E_i) = \sum_{i=1}^{n} P(E_i) - \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} P(E_i \cap E_j) + \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} \sum_{k=j+1}^{n} P(E_i \cap E_j \cap E_k) - \ldots. \tag{5.5}$$

All the sum signs in this notation suggest that we need some new notation to describe sums. We are now going to make a (hopefully small) leap of abstraction in our notation and introduce notation capable of compactly describing the sum described in the previous paragraph. This notation is an extension of the one we introduced in Equation 5.1. We use

$$\sum_{\substack{i_1, i_2, \ldots, i_k: \\ 1 \le i_1 < i_2 < \cdots < i_k \le n}} P(E_{i_1} \cap E_{i_2} \cap \cdots E_{i_k}) \tag{5.6}$$

to stand for the sum, over all sequences $i_1, i_2, \ldots i_k$ of integers between 1 and n of the probabilities of the sets $E_{i_1} \cap E_{i_2} \ldots \cap E_{i_k}$. More generally, $\sum_{\substack{i_1, i_2, \ldots, i_k: \\ 1 \le i_1 < i_2 < \cdots < i_k \le n}} f(i_1, i_2, \ldots, i_k)$ is the sum of $f(i_1, i_2, \ldots, i_k)$ over all increasing sequences of k numbers between 1 and n.

Exercise 5.2-4 To practice with notation, what is $\sum_{\substack{i_1, i_2, i_3: \\ 1 \le i_1 < i_2 < i_3 \le 4}} i_1 + i_2 + i_3$?

The sum in Exercise 5.2-4 is $1+2+3+1+2+4+1+3+4+2+3+4 = 3(1+2+3+4) = 30$.

With this understanding of the notation in hand, we can now write down a formula that captures the idea in Equation 5.5 more concisely. Notice that in Equation 5.5 we include probabilities of single sets with a plus sign, probabilities of intersections of two sets with a minus sign, and in general, probabilities of intersections of any even number of sets with a minus sign and probabilities of intersections of any odd number of sets (including the odd number one) with a plus sign. Thus if we are intersecting k sets, the proper coefficient for the probability of the intersection of these sets is $(-1)^{k+1}$ (it would be equally good to use $(-1)^{k-1}$, and correct but silly to use $(-1)^{k+3}$). This lets us translate the formula of Equation 5.5 to Equation 5.7 in the theorem, called the *Principle of Inclusion and Exclusion for Probability*, that follows. We will give two completely different proofs of the theorem, one of which is a nice counting argument but is a bit on the abstract side, and one of which is straightforward induction, but is complicated by the fact that it takes a lot of notation to say what is going on.

Theorem 5.3 (Principle of Inclusion and Exclusion for Probability) *The probability of the union $E_1 \cup E_2 \cup \cdots \cup E_n$ of events in a sample space S is given by*

$$P\left(\bigcup_{i=1}^{n} E_i\right) = \sum_{k=1}^{n} (-1)^{k+1} \sum_{\substack{i_1,i_2,\ldots,i_k: \\ 1\le i_1<i_2<\cdots<i_k\le n}} P\left(E_{i_1} \cap E_{i_2} \cap \cdots \cap E_{i_k}\right). \tag{5.7}$$

First Proof: Consider an element x of $\bigcup_{i=1}^n E_i$. Let $E_{i_1}, E_{i_2}, \ldots E_{i_k}$ be the set of all events E_i of which x is a member. Let $K = \{i_1, i_2, \ldots, i_k\}$. Then x is in the event $E_{j_1} \cap E_{j_2} \cap \cdots \cap E_{j_m}$ if and only if $\{j_1, j_2 \ldots j_m\} \subseteq K$. Why is this? If there is a j_r that is not in K, then $x \notin E_j$ and thus $x \notin E_{j_1} \cap E_{j_2} \cap \cdots \cap E_{j_m}$. Notice that every x in $\bigcup_{i=1}^n E_i$ is in at least one E_i, so it is in at least one of the sets $E_{i_1} \cap E_{i_2} \cap \cdots \cap E_{i_k}$.

Recall that we define $P\left(E_{j_1} \cap E_{j_2} \cap \cdots \cap E_{j_m}\right)$ to be the sum of the probability weights $p(x)$ for $x \in E_{j_1} \cap E_{j_2} \cap \cdots \cap E_{j_m}$. Suppose we substitute this sum of probability weights for $P\left(E_{j_1} \cap E_{j_2} \cap \cdots \cap E_{j_m}\right)$ on the right hand side of Equation 5.7. Then the right hand side becomes a sum of terms, each of which is plus or minus a probability weight. The sum of all the terms involving $p(x)$ on the right hand side of Equation 5.7 includes a term involving $p(x)$ for each nonempty subset $\{j_1, j_2, \ldots, j_m\}$ of K, and no other terms involving $p(x)$. The coefficient of the probability weight $p(x)$ in the term for the subset $\{j_1, j_2, \ldots, j_m\}$ is $(-1)^{m+1}$. Since there are $\binom{k}{m}$ subsets of K of size m, the sum of the terms involving $p(x)$ will therefore be

$$\sum_{m=1}^{k} (-1)^{m+1} \binom{k}{m} p(x) = \left(-\sum_{m=0}^{k} (-1)^m \binom{k}{m} p(x)\right) + p(x) = 0 \cdot p(x) + p(x) = p(x),$$

because $k \ge 1$ and thus by the binomial theorem, $\sum_{j=0}^{k} \binom{k}{j} (-1)^j = (1-1)^k = 0$. This proves that for each x, the sum of all the terms involving $p(x)$ after we substitute the sum of probability weights into Equation 5.7 is exactly $p(x)$. We noted above that for every x in $\cup_{i=1}^n E_i$ appears in at least one of the sets $E_{i_1} \cap E_{i_2} \cap \cdots \cap E_{i_k}$. Thus the right hand side of Equation 5.7 is the sum of every $p(x)$ such that x is in $\cup_{i=1}^n E_i$. By definition, this is the left-hand side of Equation 5.7. ■

Second Proof: The proof is simply an application of mathematical induction using Equation 5.4. When $n = 1$ the formula is true because it says $P(E_1) = P(E_1)$. Now suppose inductively that for any family of $n-1$ sets $F_1, F_2, \ldots, F_{n-1}$

$$P\left(\bigcup_{i=1}^{n-1} F_i\right) = \sum_{k=1}^{n-1} (-1)^{k+1} \sum_{\substack{i_1,i_2,i\ldots,i_k: \\ 1\le i_1<i_2<\cdots<i_k\le n-1}} P(F_{i_1} \cap F_{i_2} \cap \ldots \cap F_{i_k}) \tag{5.8}$$

If in Equation 5.4 we let $E = E_1 \cup \ldots \cup E_{n-1}$ and $F = E_m$, we may apply Equation 5.4 to to compute $P\left(\cup_{i=1}^n E_i\right)$ as follows:

$$P\left(\bigcup_{i=1}^{n} E_i\right) = P\left(\bigcup_{i=1}^{n-1} E_i\right) + P(E_n) - P\left(\left(\bigcup_{i=1}^{n-1} E_i\right) \cap E_n\right). \tag{5.9}$$

By the distributive law,

$$\left(\bigcup_{i=1}^{n-1} E_i\right) \cap E_n = \bigcup_{i=1}^{n-1} (E_i \cap E_n),$$

and substituting this into Equation 5.9 gives

$$P\left(\bigcup_{i=1}^{n} E_i\right) = P\left(\bigcup_{i=1}^{n-1} E_i\right) + P(E_n) - P\left(\bigcup_{i=1}^{n-1} (E_i \cap E_n)\right).$$

Now we use the inductive hypothesis (Equation 5.8) in two places to get

$$\begin{aligned} P\left(\bigcup_{i=1}^{n} E_i\right) &= \sum_{k=1}^{n-1} (-1)^{k+1} \sum_{\substack{i_1,i_2,i\ldots,i_k: \\ 1\le i_1<i_2<\cdots<i_k\le n-1}} P(E_{i_1} \cap E_{i_2} \cap \cdots \cap E_{i_k}) \\ &+ P(E_n) \\ &- \sum_{k=1}^{n-1} (-1)^{k+1} \sum_{\substack{i_1,i_2,i\ldots,i_k: \\ 1\le i_1<i_2<\cdots<i_k\le n-1}} P(E_{i_1} \cap E_{i_2} \cap \cdots \cap E_{i_k} \cap E_n). \end{aligned}$$

The first summation on the right hand side sums $(-1)^{k+1} P\left(E_{i_1} \cap E_{i_2} \cap \cdots \cap E_{i_k}\right)$ over all lists $i_1, i_2, \ldots, i_k$ that *do not* contain n, while the $P(E_n)$ and the second summation work together to sum $(-1)^{k+1} P\left(E_{i_1} \cap E_{i_2} \cap \cdots \cap E_{i_k}\right)$ over all lists $i_1, i_2, \ldots, i_k$ that *do* contain n. Therefore,

$$P\left(\bigcup_{i=1}^{n} E_i\right) = \sum_{k=1}^{n} (-1)^{k+1} \sum_{\substack{i_1,i_2,i\ldots,i_k: \\ 1\le i_1<i_2<\cdots<i_k\le n}} P(E_{i_1} \cap E_{i_2} \cap \cdots \cap E_{i_k}).$$

Thus by the principle of mathematical induction, this formula holds for all integers $n > 0$. ■

Exercise 5.2-5 At a fancy restaurant n students check their backpacks. They are the only ones to check backpacks. A child visits the checkroom and plays with the check tickets for the backpacks so they are all mixed up. If there are 5 students named Judy, Sam, Pat, Jill, and Jo, in how many ways may the backpacks be returned so that Judy gets her own backpack (and maybe some other students do, too)? What is the probability that this happens? What is the probability that Sam gets his backpack (and maybe some other students do, too)? What is the probability that Judy and Sam both get their own backpacks (and maybe some other students do, too)? For any particular two element set of students, what is the probability that these two students get their own backpacks (and maybe some other students do, too)? What is the probability that at least one student gets his or her own backpack? What is the probability that no students get their own backpacks? What do you expect the answer will be for the last two questions for n students? This classic problem is often stated using hats rather than backpacks (quaint, isn't it?), so it is called the *hatcheck problem*. It is also known as the *derangement problem*; a *derangement* of a set being a one-to-one function from a set onto itself (i.e., a bijection) that sends each element to something not equal to it.

For Exercise 5.2-5, let E_i be the event that person i on our list gets the right backpack. Thus E_1 is the event that Judy gets the correct backpack and E_2 is the event that Sam gets the correct backpack. The event $E_1 \cap E_2$ is the event that Judy *and* Sam get the correct backpacks (and maybe some other people do). In Exercise 5.2-5, there are 4! ways to pass back the backpacks so that Judy gets her own, as there are for Sam or any other single student. Thus $P(E_1) = P(E_i) = \frac{4!}{5!}$. For any particular two element subset, such as Judy and Sam, there are 3! ways that these two people may get their backpacks back. Thus, for each i and j, $P(E_i \cap E_j) = \frac{3!}{5!}$. For a particular group of k students the probability that each one of these k students gets his or her own backpack back is $(5-k)!/5!$. If E_i is the event that student i gets his or her own backpack back, then the probability of an intersection of k of these events is $(5-k)!/5!$. The probability that at least one person gets his or her own backpack back is the probability of $E_1 \cup E_2 \cup E_3 \cup E_4 \cup E_5$. Then by the principle of inclusion and exclusion, the probability that at least one person gets his or her own backpack back is

$$P(E_1 \cup E_2 \cup E_3 \cup E_4 \cup E_5) = \sum_{k=1}^{5} (-1)^{k+1} \sum_{\substack{i_1, i_2, \ldots, i_k:\\ 1 \le i_1 < i_2 < \cdots < i_k \le 5}} P(E_{i_1} \cap E_{i_2} \cap \cdots \cap E_{i_k}). \tag{5.10}$$

As we argued above, for a set of k people, the probability that all k people get their backpacks back is $(5-k)!/5!$. In symbols, $P(E_{i_1} \cap E_{i_2} \cap \cdots \cap E_{i_k}) = \frac{(5-k)!}{5!}$. Recall that there are $\binom{5}{k}$ sets of k people chosen from our five students. That is, there are $\binom{5}{k}$ lists $i_1, i_2, \ldots i_k$ with $1 < i_1 < i_2 < \cdots < i_k \le 5$. Thus, we can rewrite the right hand side of the Equation 5.10 as

$$\sum_{k=1}^{5} (-1)^{k+1} \binom{5}{k} \frac{(5-k)!}{5!}.$$

This gives us

$$\begin{aligned}
P(E_1 \cup E_2 \cup E_3 \cup E_4 \cup E_5) &= \sum_{k=1}^{5} (-1)^{k-1} \binom{5}{k} \frac{(5-k)!}{5!} \\
&= \sum_{k=1}^{5} (-1)^{k-1} \frac{5!}{k!(5-k)!} \frac{(5-k)!}{5!} \\
&= \sum_{k=1}^{5} (-1)^{k-1} \frac{1}{k!} \\
&= 1 - \frac{1}{2} + \frac{1}{3!} - \frac{1}{4!} + \frac{1}{5!}.
\end{aligned}$$

The probability that nobody gets his or her own backpack is 1 minus the probability that someone does, or

$$\frac{1}{2} - \frac{1}{3!} + \frac{1}{4!} - \frac{1}{5!}.$$

To do the general case of n students, we simply substitute n for 5 and get that the probability that at least one person gets his or her own backpack is

$$\sum_{i=1}^{n}(-1)^{i-1}\frac{1}{i!} = 1 - \frac{1}{2} + \frac{1}{3!} - \cdots + \frac{(-1)^{n-1}}{n!}$$

and the probability that nobody gets his or her own backpack is 1 minus the probability above, or

$$\sum_{i=2}^{n}(-1)^{i}\frac{1}{i!} = \frac{1}{2} - \frac{1}{3!} + \cdots + \frac{(-1)^{n}}{n!}. \tag{5.11}$$

Those who have had power series in calculus may recall the power series representation of e^x, namely

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots = \sum_{i=0}^{\infty}\frac{x^i}{i!}.$$

Thus the expression in Equation 5.11 is the approximation to e^{-1} we get by substituting -1 for x in the power series and stopping the series at $i = n$. Note that the result depends very "lightly" on n; so long as we have at least four or five people, then, no matter how many people we have, the probability that no one gets their hat back remains at roughly e^{-1}. Our intuition might have suggested that as the number of students increases, the probability that *someone* gets his or her own backpack back approaches 1 rather than $1 - e^{-1}$. Here is another example of why it is important to use computations with the rules of probability instead of intuition!

The principle of inclusion and exclusion for counting

Exercise 5.2-6 How many functions are there from an n-element set N to a k-element set $K = \{y_1, y_2, \ldots y_k\}$ that map nothing to y_1? Another way to say this is if I have n distinct candy bars and k children Sam, Mary, Pat, etc., in how ways may I pass out the candy bars so that Sam doesn't get any candy (and maybe some other children don't either)?

Exercise 5.2-7 How many functions map nothing to a j-element subset J of K? Another way to say this is if I have n distinct candy bars and k children Sam, Mary, Pat, etc., in how ways may I pass out the candy bars so that some particular j-element subset of the children don't get any (and maybe some other children don't either)?

Exercise 5.2-8 What is the number of functions from an n-element set N to a k element set K that map nothing to at least one element of K? Another way to say this is if I have n distinct candy bars and k children Sam, Mary, Pat, etc., in how ways may I pass out the candy bars so that some child doesn't get any (and maybe some other children don't either)?

Exercise 5.2-9 On the basis of the previous exercises, how many functions are there from an n-element set onto a k element set?

The number of functions from an n-element set to a k-element set $K = \{y_1, y_2, \ldots y_k\}$ that map nothing to y_1 is simply $(k-1)^n$ because we have $k-1$ choices of where to map each of our n elements. Similarly the number of functions that map nothing to a particular set J of j elements will be $(k-j)^n$. This warms us up for Exercise 5.2-8.

In Exercise 5.2-8 we need an analog of the principle of inclusion and exclusion for the size of a union of k sets (set i being the set of functions that map nothing to element i of the set K). Because we can make the same argument about the size of the union of two or three sets that we made about probabilities of unions of two or three sets, we have a very natural analog. That analog is the *Principle of Inclusion and Exclusion for Counting*

$$\left|\bigcup_{i=1}^{n} E_i\right| = \sum_{k=1}^{n}(-1)^{k+1} \sum_{\substack{i_1,i_2,\ldots,i_k:\\ 1\le i_1<i_2<\cdots<i_k\le n}} \left|E_{i_1} \cap E_{i_2} \cap \cdots \cap E_{i_k}\right|. \tag{5.12}$$

In fact, this formula is proved by induction or a counting argument in virtually the same way. Applying this formula to the number of functions from N that map nothing to at least one element of K gives us

$$|\bigcup_{i=1}^{k} E_i| = \sum_{k=1}^{n}(-1)^{k+1} \sum_{\substack{i_1,i_2,\ldots,i_k:\\ 1\le i_1<i_2<\cdots<i_k\le n}} |E_{i_1} \cap E_{i_2} \cap \cdots \cap E_{i_k}| = \sum_{j=1}^{k}(-1)^{j-1}\binom{k}{j}(k-j)^n.$$

This is the number of functions from N that map nothing to at least one element of K. The total number of functions from N to K is k^n. Thus the number of onto functions is

$$k^n - \sum_{j=1}^{k}(-1)^{j-1}\binom{k}{j}(k-j)^n = \sum_{j=0}^{k}(-1)^{j}\binom{k}{j}(k-j)^n,$$

where the second equality results because $\binom{k}{0}$ is 1 and $(k-0)^n$ is k^n.

Important Concepts, Formulas, and Theorems

1. *Venn Diagram.* To draw a *Venn diagram*, for two or three sets, we draw a rectangle that represents the sample space, and two or three mutually overlapping circles to represent the events.

2. *Probability of a Union of Two Events.* $P(E \cup F) = P(E) + P(F) - P(E \cap F)$

3. *Probability of a Union of Three Events.* $P(E \cup F \cup G) = P(E) + P(F) + P(G) - P(E \cap F) - P(E \cap G) - P(F \cap G) + P(E \cap F \cap G)$.

4. *A Summation Notation.* $\displaystyle\sum_{\substack{i_1,i_2,\ldots,i_k:\\ 1\le i_1<i_2<\cdots<i_k\le n}} f(i_1, i_2, \ldots, i_k)$ is the sum of $f(i_1, i_2, \ldots, i_k)$ over all increasing sequences of k numbers between 1 and n.

5. *Principle of Inclusion and Exclusion for Probability.* The probability of the union $E_1 \cup E_2 \cup \cdots \cup E_n$ of events in a sample space S is given by

$$P\left(\bigcup_{i=1}^{n} E_i\right) = \sum_{k=1}^{n}(-1)^{k+1} \sum_{\substack{i_1,i_2,\ldots,i_k:\\ 1\le i_1<i_2<\cdots<i_k\le n}} P\left(E_{i_1} \cap E_{i_2} \cap \cdots \cap E_{i_k}\right).$$

6. *Hatcheck Problem.* The *hatcheck problem* or *derangement problem* asks for the probability that a bijection of an n element set maps no element to itself. The answer is

$$\sum_{i=2}^{n}(-1)^i\frac{1}{i!} = \frac{1}{2} - \frac{1}{3!} + \cdots + \frac{(-1)^n}{n!},$$

the result of truncating the power series expansion of e^{-1} at the $\frac{(-1)^n}{n!}$. Thus the result is very close to $\frac{1}{e}$, even for relatively small values of n.

7. *Principle of Inclusion and Exclusion for Counting.* The *Principle of inclusion and exclusion for counting* says that

$$\left|\bigcup_{i=1}^{n} E_i\right| = \sum_{k=1}^{n}(-1)^{k+1} \sum_{\substack{i_1,i_2,\ldots,i_k:\\ 1\le i_1<i_2<\cdots<i_k\le n}} \left|E_{i_1} \cap E_{i_2} \cap \cdots \cap E_{i_k}\right|.$$

Problems

1. Compute the probability that in three flips of a coin the coin comes heads on the first flip or on the last flip.

2. The eight kings and queens are removed from a deck of cards and then two of these cards are selected. What is the probability that the king or queen of spades is among the cards selected?

3. Two dice are rolled. What is the probability that we see a die with six dots on top?

4. A bowl contains two red, two white and two blue balls. We remove two balls. What is the probability that at least one is red or white? Compute the probability that at least one is red.

5. From an ordinary deck of cards, we remove one card. What is the probability that it is an Ace, is a diamond, or is black?

6. Give a formula for the probability of $P(E \cup F \cup G \cup H)$ in terms of the probabilities of E,F, G, and H, and their intersections.

7. What is

$$\sum_{\substack{i_1,i_2,i_3:\\ 1\le i_1<i_2<i_3\le 4}} i_1 i_2 i_3 \text{ ?}$$

8. What is

$$\sum_{\substack{i_1,i_2,i_3:\\ 1\le i_1<i_2<i_3\le 5}} i_1 + i_2 + i_3 \text{ ?}$$

9. The boss asks the secretary to stuff n letters into envelopes forgetting to mention that he has been adding notes to the letters and in the process has rearranged the letters but not the envelopes. In how many ways can the letters be stuffed into the envelopes so that nobody gets the letter intended for him or her? What is the probability that nobody gets the letter intended for him or her?

10. If we are hashing n keys into a hash table with k locations, what is the probability that every location gets at least one key?

11. From the formula for the number of onto functions, find a formula for $S(n, k)$ which is defined in Problem 12 of Section 1.4. These numbers are called *Stirling numbers (of the second kind)*.

12. If we roll 8 dice, what is the probability that each of the numbers 1 through 6 appear on top at least once? What about with 9 dice?

13. Explain why the number of ways of distributing k identical apples to n children is $\binom{n+k-1}{k}$. In how many ways may you distribute the apples to the children so that Sam gets more than m? In how many ways may you distribute the apples to the children so that no child gets more than m?

14. A group of n married couples sits a round a circular table for a group discussion of marital problems. The counselor assigns each person to a seat at random. What is the probability that no husband and wife are side by side?

15. Suppose we have a collection of m objects and a set P of p "properties," an undefined term, that the objects may or may not have. For each subset S of the set P of all properties, define $N_a(S)$ (a is for "at least") to be the number of objects in the collection that have at least the properties in S. Thus, for example, $N_a(\emptyset) = m$. In a typical application, formulas for $N_a(S)$ for other sets $S \subseteq P$ are not difficult to figure out. Define $N_e(S)$ to be the number of objects in our collection that have exactly the properties in S. Show that

$$N_e(\emptyset) = \sum_{K: K \subseteq P} (-1)^{|K|} N_a(K).$$

Explain how this formula could be used for computing the number of onto functions in a more direct way than we did it using unions of sets. How would this formula apply to Problem 9 in this section?

16. In Problem 14 of this section we allow two people of the same sex to sit side by side. If we require in addition to the condition that no husband and wife are side by side the condition that no two people of the same sex are side by side, we obtain a famous problem known as the *mènage* problem. Solve this problem.

17. In how many ways may we place n distinct books on j shelves so that shelf one gets at least m books? (See Problem 7 in Section 1.4.) In how many ways may we place n distinct books on j shelves so that no shelf gets more than m books?

18. In Problem 15 in this section, what is the probability that an object has none of the properties, assuming all objects to be equally likely? How would this apply Problem 10 in this section?

5.3 Conditional Probability and Independence

Conditional Probability

Two cubical dice each have a triangle painted on one side, a circle painted on two sides and a square painted on three sides. Applying the principal of inclusion and exclusion, we can compute that the probability that we see a circle on at least one top when we roll them is $1/3 + 1/3 - 1/9 = 5/9$. We are experimenting to see if reality agrees with our computation. We throw the dice onto the floor and they bounce a few times before landing in the next room.

Exercise 5.3-1 Our friend in the next room tells us both top sides are the same. Now what is the probability that our friend sees a circle on at least one top?

Intuitively, it may seem as if the chance of getting circles ought to be four times the chance of getting triangles, and the chance of getting squares ought to be nine times as much as the chance of getting triangles. We could turn this into the algebraic statements that $P(\text{circles}) = 4P(\text{triangles})$ and $P(\text{squares}) = 9P(\text{triangles})$. These two equations and the fact that the probabilities sum to 1 would give us enough equations to conclude that the probability that our friend saw two circles is now $2/7$. But does this analysis make sense? To convince ourselves, let us start with a sample space for the original experiment and see what natural assumptions about probability we can make to determine the new probabilities. In the process, we will be able to replace intuitive calculations with a formula we can use in similar situations. This is a good thing, because we have already seen situations where our intuitive idea of probability might not always agree with what the rules of probability give us.

Let us take as our sample space for this experiment the ordered pairs shown in Table 5.2 along with their probabilities.

Table 5.2: Rolling two unusual dice

TT	TC	TS	CT	CC	CS	ST	SC	SS
$\frac{1}{36}$	$\frac{1}{18}$	$\frac{1}{12}$	$\frac{1}{18}$	$\frac{1}{9}$	$\frac{1}{6}$	$\frac{1}{12}$	$\frac{1}{6}$	$\frac{1}{4}$

We know that the event {TT, CC, SS} happened. Thus we would say while it used to have probability

$$\frac{1}{36} + \frac{1}{9} + \frac{1}{4} = \frac{14}{36} = \frac{7}{18} \tag{5.13}$$

this event now has probability 1. Given that, what probability would we now assign to the event of seeing a circle? Notice that the event of seeing a circle now has become the event CC. Should we expect CC to become more or less likely in comparison than TT or SS just because we know now that one of these three outcomes has occurred? Nothing has happened to make us expect that, so whatever new probabilities we assign to these two events, they should have the same ratios as the old probabilities.

Multiplying all three old probabilities by $\frac{18}{7}$ to get our new probabilities will preserve the ratios and make the three new probabilities add to 1. (Is there any other way to get the three new probabilities to add to one and make the new ratios the same as the old ones?) This gives us that the probability of two circles is $\frac{1}{9} \cdot \frac{18}{7} = \frac{2}{7}$. Notice that nothing we have learned about probability so far told us what to do; we just made a decision based on common sense. When faced with similar situations in the future, it would make sense to use our common sense in the same way. However, do we really need to go through the process of constructing a new sample space and reasoning about its probabilities again? Fortunately, our entire reasoning process can be captured in a formula. We wanted the probability of an event E given that the event F happened. We figured out what the event $E \cap F$ was, and then multiplied its probability by $1/P(F)$. We summarize this process in a definition.

We define the *conditional probability* of E given F, denoted by $P(E|F)$ and read as "the probability of E given F" by

$$P(E|F) = \frac{P(E \cap F)}{P(F)}. \tag{5.14}$$

Then whenever we want the probability of E knowing that F has happened, we compute $P(E|F)$. (If $P(F) = 0$, then we cannot divide by $P(F)$, but F gives us no new information about our situation. For example if the student in the next room says "A pentagon is on top," we have no information except that the student isn't looking at the dice we rolled! Thus we have no reason to change our sample space or the probability weights of its elements, so we define $P(E|F) = P(E)$ when $P(F) = 0$.)

Notice that we did not prove that the probability of E given F is what we said it is; we simply defined it in this way. That is because in the process of making the derivation we made an additional assumption that the relative probabilities of the outcomes in the event F don't change when F happens. This assumption led us to Equation 5.14. Then we chose that equation as our definition of the new concept of the conditional probability of E given F.[4]

In the example above, we can let E be the event that there is more than one circle and F be the event that both dice are the same. Then $E \cap F$ is the event that both dice are circles, and $P(E \cap F)$ is, from the table above, $\frac{1}{9}$. $P(F)$ is, from Equation 5.13, $\frac{7}{18}$. Dividing, we get the probability of $P(E|F)$, which is $\frac{1}{9}/\frac{7}{18} = \frac{2}{7}$.

Exercise 5.3-2 When we roll two ordinary dice, what is the probability that the sum of the tops comes out even, given that the sum is greater than or equal to 10? Use the definition of conditional probability in solving the problem.

Exercise 5.3-3 We say E is *independent* of F if $P(E|F) = P(E)$. Show that when we roll two dice, one red and one green, the event "The total number of dots on top is odd" is independent of the event "The red die has an odd number of dots on top."

Exercise 5.3-4 Sometimes information about conditional probabilities is given to us indirectly in the statement of a problem, and we have to derive information about other probabilities or conditional probabilities. Here is such an example. If a student knows 80% of the material in a course, what do you expect her grade to be on a (well-balanced) 100 question short-answer test about the course? What is the probability that she answers a question correctly on a 100 question true-false test if she guesses at each question she does not know the answer to? (We assume that she knows what

[4]For those who like to think in terms of axioms of probability, we could give an axiomatic definition of conditional probability, and one of our axioms might be that for events E_1 and E_2 that are subsets of F, the ratio of the conditional probabilities $P(E_1|F)$ and $P(E_2|F)$ is the same as the ratio of $P(E_1)$ and $P(E_2)$.

she knows, that is, if she thinks that she knows the answer, then she really does.) What do you expect her grade to be on a 100 question True-False test to be?

For Exercise 5.3-2 let's let E be the event that the sum is even and F be the event that the sum is greater than or equal to 10. Thus referring to our sample space in Exercise 5.3-2, $P(F) = 1/6$ and $P(E \cap F) = 1/9$, since it is the probability that the roll is either 10 or 12. Dividing these two we get 2/3.

In Exercise 5.3-3, the event that the total number of dots is odd has probability 1/2. Similarly, given that the red die has an odd number of dots, the probability of an odd sum is 1/2 since this event corresponds exactly to getting an even roll on the green die. Thus, by the definition of independence, the event of an odd number of dots on the red die and the event that the total number of dots is odd are independent.

In Exercise 5.3-4, if a student knows 80% of the material in a course, we would hope that her grade on a well-designed test of the course would be around 80%. But what if the test is a True-False test? Let R be the event that she gets the right answer, K be the event that she knows that right answer and $\overline{K}$ be the event that she guesses. Then $R = P(R \cap K) + P(R \cap \overline{K})$. Since R is a union of two disjoint events, its probability would be the sum of the probabilities of these two events. How do we get the probabilities of these two events? The statement of the problem gives us implicitly the conditional probability that she gets the right answer given that she knows the answer, namely one, and the probability that she gets the right answer if she doesn't know the answer, namely 1/2. Using Equation 5.14, we see that we use the equation

$$P(E \cap F) = P(E|F)P(F) \tag{5.15}$$

to compute $P(R \cap K)$ and $P(R \cap \overline{K})$, since the problem tells us directly that $P(K) = .8$ and $P(\overline{K}) = .2$. In symbols,

$$\begin{aligned} P(R) &= P(R \cap K) + P(R \cap \overline{K}) \\ &= P(R|K)P(K) + P(R|\overline{K})P(\overline{K}) \\ &= 1 \cdot .8 + .5 \cdot .2 = .9. \end{aligned}$$

We have shown that the probability that she gets the right answer is .9. Thus we would expect her to get a grade of 90%.

Independence

We said in Exercise 5.3-3 that E is independent of F if $P(E|F) = P(E)$. The *product principle for independent probabilities* (Theorem 5.4) gives another test for independence.

Theorem 5.4 *Suppose E and F are events in a sample space. Then E is independent of F if and only if $P(E \cap F) = P(E)P(F)$.*

Proof: First consider the case when F is non-empty. Then, from our definition in Exercise 5.3-3

$$E \text{ is independent of } F \quad \Leftrightarrow \quad P(E|F) = P(E).$$

(Even though the definition only has an "if", recall the convention of using "if" in definitions, even though "if and only if" is meant.) Using the definition of $P(E|F)$ in Equation 5.14, in the right side of the above equation we get

$$\begin{aligned} & P(E|F) = P(E) \\ \Leftrightarrow\quad & \frac{P(E\cap F)}{P(F)} = P(E) \\ \Leftrightarrow\quad & P(E\cap F) = P(E)P(F). \end{aligned}$$

Since every step in this proof was an if and only if statement we have completed the proof for the case when F is non-empty.

If F is empty, then E is independent of F and both $P(E)P(F)$ and $P(E\cap F)$ are zero. Thus in this case as well, E is independent of F if and only if $P(E\cap F) = P(E)P(F)$. ■

Corollary 5.5 *E is independent of F if and only if F is independent of E.*

When we flip a coin twice, we think of the second outcome as being independent of the first. It would be a sorry state of affairs if our definition of independence did not capture this intuitive idea! Let's compute the relevant probabilities to see if it does. For flipping a coin twice our sample space is $\{HH, HT, TH, TT\}$ and we weight each of these outcomes 1/4. To say the second outcome is independent of the first, we must mean that getting an H second is independent of whether we get an H or a T first, and same for getting a T second. This gives us that $P(H \text{ first}) = 1/4+1/4 = 1/2$ and $P(H \text{ second}) = 1/2$, while $P(\text{H first and H second}) = 1/4$. Note that

$$P(H \text{ first})P(H \text{ second}) = \frac{1}{2}\cdot\frac{1}{2} = \frac{1}{4} = P(\text{H first and H second}).$$

By Theorem 5.4, this means that the event "H second" is independent of the event"H first." We can make a similar computation for each possible combination of outcomes for the first and second flip, and so we see that our definition of independence captures our intuitive idea of independence in this case. Clearly the same sort of computation applies to rolling dice as well.

Exercise 5.3-5 What sample space and probabilities have we been using when discussing hashing? Using these, show that the event "key i hashes to position p" and the event "key j hashes to position q" are independent when $i \neq j$. Are they independent if $i = j$?

In Exercise 5.3-5 if we have a list of n keys to hash into a table of size k, our sample space consists of all n-tuples of numbers between 1 and k. The event that key i hashes to some number p consists of all n-tuples with p in the ith position, so its probability is $\left(\frac{1}{k}\right)^{n-1}/\left(\frac{1}{k}\right)^{n} = \frac{1}{k}$. The probability that key j hashes to some number q is also $\frac{1}{k}$. If $i \neq j$, then the event that key i hashes to p and key j hashes to q has probability $\left(\frac{1}{k}\right)^{n-2}/\left(\frac{1}{k}\right)^{n} = \left(\frac{1}{k}\right)^{2}$, which is the product of the probabilities that key i hashes to p and key j hashes to q, so these two events are independent. However if $i = j$ the probability of key i hashing to p and key j hashing to q is zero unless $p = q$, in which case it is 1. Thus if $i = j$, these events are not independent.

Independent Trials Processes

Coin flipping and hashing are examples of what are called "independent trials processes." Suppose we have a process that occurs in stages. (For example, we might flip a coin n times.) Let us use x_i to denote the outcome at stage i. (For flipping a coin n times, $x_i = H$ means that the outcome of the ith flip is a head.) We let S_i stand for the set of possible outcomes of stage i. (Thus if we flip a coin n times, $S_i = \{H, T\}$.) A process that occurs in stages is called an **independent trials process** if for each sequence $a_1, a_2, \ldots, a_n$ with $a_i \in S_i$,

$$P(x_i = a_i | x_1 = a_1, \ldots, x_{i-1} = a_{i-1}) = P(x_i = a_i).$$

In other words, if we let E_i be the event that $x_i = a_i$, then

$$P(E_i | E_1 \cap E_2 \cap \cdots \cap E_{i-1}) = P(E_i).$$

By our product principle for independent probabilities, this implies that

$$P(E_1 \cap E_2 \cap \cdots E_{i-1} \cap E_i) = P(E_1 \cap E_2 \cap \cdots E_{i-1}) P(E_i). \tag{5.16}$$

Theorem 5.6 *In an independent trials process the probability of a sequence $a_1, a_2, \ldots, a_n$ of outcomes is $P(\{a_1\})P(\{a_2\}) \cdots P(\{a_n\})$.*

Proof: We apply mathematical induction and Equation 5.16. ■

How do independent trials relate to coin flipping? Here our sample space consists of sequences of n Hs and Ts, and the event that we have an H (or T) on the ith flip is independent of the event that we have an H (or T) on each of the first $i-1$ flips. In particular, the probability of an H on the ith flip is $2^{n-1}/2^n = .5$, and the probability of an H on the ith flip, given a particular sequence on the first $i-1$ flips is $2^{n-i-1}/2^{n-i} = .5$.

How do independent trials relate to hashing a list of keys? As in Exercise 5.3-5 if we have a list of n keys to hash into a table of size k, our sample space consists of all n-tuples of numbers between 1 and k. The probability that key i hashes to p and keys 1 through $i-1$ hash to q_1, q_2,… q_{i-1} is $\left(\frac{1}{k}\right)^{n-i} / \left(\frac{1}{k}\right)^n$ and the probability that keys 1 through $i-1$ hash to q_1, q_2,… q_{i-1} is $\left(\frac{1}{k}\right)^{n-i+1} / \left(\frac{1}{k}\right)^n$. Therefore

$$P(\text{key } i \text{ hashes to } p | \text{keys 1 through } i-1 \text{ hash to } q_1,\ q_2,\ldots q_{i-1}) = \frac{\left(\frac{1}{k}\right)^{n-i} / \left(\frac{1}{k}\right)^n}{\left(\frac{1}{k}\right)^{n-i+1} / \left(\frac{1}{k}\right)^n} = \frac{1}{k}.$$

Therefore, the event that key i hashes to some number p is independent of the event that the first $i-1$ keys hash to some numbers q_1, q_2,… q_{i-1}. Thus our model of hashing is an independent trials process.

Exercise 5.3-6 Suppose we draw a card from a standard deck of 52 cards, replace it, draw another card, and continue for a total of ten draws. Is this an independent trials process?

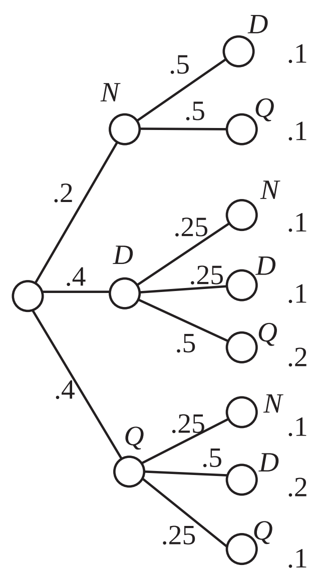
Exercise 5.3-7 Suppose we draw a card from a standard deck of 52 cards, discard it (i.e. we do not replace it), draw another card and continue for a total of ten draws. Is this an independent trials process?

In Exercise 5.3-6 we have an independent trials process, because the probability that we draw a given card at one stage does not depend on what cards we have drawn in earlier stages. However, in Exercise 5.3-7, we don't have an independent trials process. In the first draw, we have 52 cards to draw from, while in the second draw we have 51. In particular, we do not have the same cards to draw from on the second draw as the first, so the probabilities for each possible outcome on the second draw depend on whether that outcome was the result of the first draw.

Tree diagrams

When we have a sample space that consists of sequences of outcomes, it is often helpful to visualize the outcomes by a tree diagram. We will explain what we mean by giving a tree diagram of the following experiment. We have one nickel, two dimes, and two quarters in a cup. We draw a first and second coin. In Figure 5.3 you see our diagram for this process. Notice that in probability theory it is standard to have trees open to the right, rather than opening up or down.

Figure 5.5: A tree diagram illustrating a two-stage process.



Each level of the tree corresponds to one stage of the process of generating a sequence in our sample space. Each vertex is labeled by one of the possible outcomes at the stage it represents. Each edge is labeled with a conditional probability, the probability of getting the outcome at its right end given the sequence of outcomes that have occurred so far. Since no outcomes have occurred at stage 0, we label the edges from the root to the first stage vertices with the probabilities of the outcomes at the first stage. Each path from the root to the far right of the tree represents a possible sequence of outcomes of our process. We label each leaf node with the probability of the sequence that corresponds to the path from the root to that node. By the definition of conditional probabilities, the probability of a path is the product of the probabilities along its edges. We draw a probability tree for any (finite) sequence of successive trials in this way.

Sometimes a probability tree provides a very effective way of answering questions about a process. For example, what is the probability of having a nickel in our coin experiment? We see there are four paths containing an N, and the sum of their weights is .4, so the probability that one of our two coins is a nickel is .4.

Exercise 5.3-8 How can we recognize from a probability tree whether it is the probability tree of an independent trials process?

Exercise 5.3-9 In Exercise 5.3-4 we asked (among other things), if a student knows 80% of the material in a course, what is the probability that she answers a question correctly on a 100 question True-False test (assuming that she guesses on any question she does not know the answer to)? (We assume that she knows what she knows, that is, if she thinks that she knows the answer, then she really does.) Show how we can use a probability tree to answer this question.

Exercise 5.3-10 A test for a disease that affects 0.1% of the population is 99% effective on people with the disease (that is, it says they have it with probability 0.99). The test gives a false reading (saying that a person who does not have the disease is affected with it) for 2% of the population without the disease. We can think of choosing someone and testing them for the disease as a two stage process. In stage 1, we either choose someone with the disease or we don't. In stage two, the test is either positive or it isn't. Give a probability tree for this process. What is the probability that someone selected at random and given a test for the disease will have a positive test? What is the probability that someone who has positive test results in fact has the disease?

A tree for an independent trials process has the property that at each level, for each node at that level, the (labeled) tree consisting of that node and all its children is identical to each labeled tree consisting of another node at that level and all its children. If we have such a tree, then it automatically satisfies the definition of an independent trials process.

In Exercise 5.3-9, if a student knows 80% of the material in a course, we expect that she has probability .8 of knowing the answer to any given question of a well-designed true-false test. We regard her work on a question as a two stage process; in stage 1 she determines whether she knows the answer, and in stage 2, she either answers correctly with probability 1, or she guesses, in which case she answers correctly with probability 1/2 and incorrectly with probability 1/2. Then as we see in Figure 5.3 there are two root-leaf paths corresponding to her getting a correct answer. One of these paths has probability .8 and the other has probability .1. Thus she actually has probability .9 of getting a right answer if she guesses at each question she does not know the answer to.

In Figure 5.3 we show the tree diagram for thinking of Exercise 5.3-10 as a two stage process. In the first stage, a person either has or doesn't have the disease. In the second stage we administer the test, and its result is either positive or not. We use D to stand for having the disease and ND to stand for not having the disease. We use "pos" to stand for a positive test and "neg" to stand for a negative test, and assume a test is either positive or negative. The question asks us for the conditional probability that someone has the disease, given that they test positive. This is

$$P(D|\text{pos}) = \frac{P(D \cap \text{pos})}{P(\text{pos})}.$$

Figure 5.6: The probability of getting a right answer is .9.

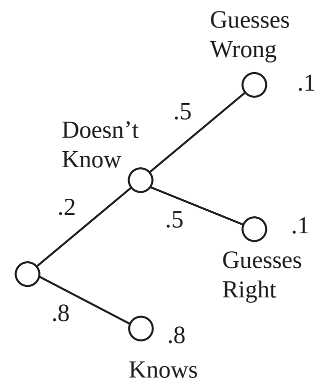
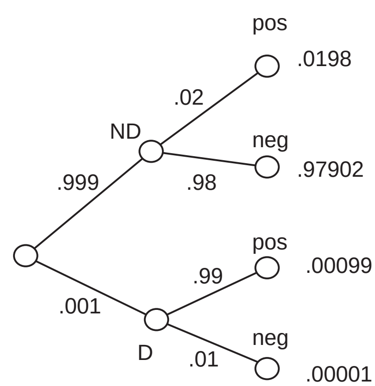


Figure 5.7: A tree diagram illustrating Exercise 5.3-10.



From the tree, we read that $P(D \cap \text{pos}) = .00099$ because this event consists of just one root-leaf path. The event "pos" consists of two root-leaf paths whose probabilities total $.0198 + .00099 = .02097$. Thus $P(D|\text{pos}) = P(D \cap \text{pos})/P(\text{pos}) = .00099/.02097 = .0472$. Thus, given a disease this rare and a test with this error rate, a positive result only gives you roughly a 5% chance of having the disease! Here is another instance where a probability analysis shows something we might not have expected initially. This explains why doctors often don't want to administer a test to someone unless that person is already showing some symptoms of the disease being tested for.

We can also do Exercise 5.3-10 purely algebraically. We are given that

$$P(\text{disease}) = .001, \tag{5.17}$$
$$P(\text{positive test result}|\text{disease}) = .99, \tag{5.18}$$
$$P(\text{positive test result}|\text{no disease}) = .02. \tag{5.19}$$

We wish to compute

$$P(\text{disease}|\text{positive test result}).$$

We use Equation 5.14 to write that

$$P(\text{disease}|\text{positive test result}) = \frac{P(\text{disease} \cap \text{positive test result})}{P(\text{positive test result})}. \tag{5.20}$$

How do we compute the numerator? Using the fact that $P(\text{disease} \cap \text{positive test result}) = P(\text{positive test result} \cap \text{disease})$ and Equation 5.14 again, we can write

$$P(\text{positive test result}|\text{disease}) = \frac{P(\text{positive test result} \cap \text{disease})}{P(\text{disease})}.$$

Plugging Equations 5.18 and 5.17 into this equation, we get

$$.99 = \frac{P(\text{positive test result} \cap \text{disease})}{.001}$$

or $P(\text{positive test result} \cap \text{disease}) = (.001)(.99) = .00099$.

To compute the denominator of Equation 5.20, we observe that since each person either has the disease or doesn't, we can write

$$P(\text{positive test}) = P(\text{positive test} \cap \text{disease}) + P(\text{positive test} \cap \text{no disease}). \tag{5.21}$$

We have already computed $P(\text{positive test result} \cap \text{disease})$, and we can compute the probability $P(\text{positive test result} \cap \text{no disease})$ in a similar manner. Writing

$$P(\text{positive test result}|\text{no disease}) = \frac{P(\text{positive test result} \cap \text{no disease})}{P(\text{no disease})},$$

observing that $P(\text{no disease}) = 1 - P(\text{disease})$ and plugging in the values from Equations 5.17 and 5.19, we get that $P(\text{positive test result} \cap \text{no disease}) = (.02)(1 - .001) = .01998$ We now have the two components of the right hand side of Equation 5.21 and thus $P(\text{positive test result}) = .00099 + .01998 = .02097$. Finally, we have all the pieces in Equation 5.20, and conclude that

$$P(\text{disease}|\text{positive test result}) = \frac{P(\text{disease} \cap \text{positive test result})}{P(\text{positive test result})} = \frac{.00099}{.02097} = .0472.$$

Clearly, using the tree diagram mirrors these computations, but it both simplifies the thought process and reduces the amount we have to write.

Important Concepts, Formulas, and Theorems

1. *Conditional Probability.* We define the *conditional probability* of E given F, denoted by $P(E|F)$ and read as "the probability of E given F" to be
$$P(E|F) = \frac{P(E \cap F)}{P(F)}.$$

2. *Independent.* We say E is *independent* of F if $P(E|F) = P(E)$.

3. *Product Principle for Independent Probabilities.* The *product principle for independent probabilities* (Theorem 5.4) gives another test for independence. Suppose E and F are events in a sample space. Then E is independent of F if and only if $P(E \cap F) = P(E)P(F)$.

4. *Symmetry of Independence.* The event E is independent of the event F if and only if F is independent of E.

5. *Independent Trials Process.* A process that occurs in stages is called an *independent trials process* if for each sequence $a_1, a_2, \ldots, a_n$ with $a_i \in S_i$,

$$P(x_i = a_i | x_1 = a_1, \ldots, x_{i-1} = a_{i-1}) = P(x_i = a_i).$$

6. *Probabilities of Outcomes in Independent Trials.* In an independent trials process the probability of a sequence $a_1, a_2, \ldots, a_n$ of outcomes is $P(\{a_1\})P(\{a_2\}) \cdots P(\{a_n\})$.

7. *Coin Flipping.* Repeatedly flipping a coin is an independent trials process.

8. *Hashing.* Hashing a list of n keys into k slots is an independent trials process with n stages.

9. *Probability Tree.* In a probability tree for a multistage process, each level of the tree corresponds to one stage of the process. Each vertex is labeled by one of the possible outcomes at the stage it represents. Each edge is labeled with a conditional probability, the probability of getting the outcome at its right end given the sequence of outcomes that have occurred so far. Each path from the root to a leaf represents a sequence of outcomes and is labelled with the product of the probabilities along that path. This is the probability of that sequence of outcomes.

Problems

1. In three flips of a coin, what is the probability that two flips in a row are heads, given that there is an even number of heads?

2. In three flips of a coin, is the event that two flips in a row are heads independent of the event that there is an even number of heads?

3. In three flips of a coin, is the event that we have at most one tail independent of the event that not all flips are identical?

4. What is the sample space that we use for rolling two dice, a first one and then a second one? Using this sample space, explain why it is that if we roll two dice, the event "i dots are on top of the first die" and the event "j dots are on top of the second die" are independent.

5. If we flip a coin twice, is the event of having an odd number of heads independent of the event that the first flip comes up heads? Is it independent of the event that the second flip comes up heads? Would you say that the three events are mutually independent? (This hasn't been defined, so the question is one of opinion. However you should back up your opinion with a reason that makes sense!)

6. Assume that on a true-false test, students will answer correctly any question on a subject they know. Assume students guess at answers they do not know. For students who know 60% of the material in a course, what is the probability that they will answer a question correctly? What is the probability that they will know the answer to a question they answer correctly?

7. A nickel, two dimes, and two quarters are in a cup. We draw three coins, one at a time, without replacement. Draw the probability tree which represents the process. Use the tree to determine the probability of getting a nickel on the last draw. Use the tree to determine the probability that the first coin is a quarter, given that the last coin is a quarter.

8. Write down a formula for the probability that a bridge hand (which is 13 cards, chosen from an ordinary deck) has four aces, given that it has one ace. Write down a formula for the probability that a bridge hand has four aces, given that it has the ace of spades. Which of these probabilities is larger?

9. A nickel, two dimes, and three quarters are in a cup. We draw three coins, one at a time without replacement. What is the probability that the first coin is a nickel? What is the probability that the second coin is a nickel? What is the probability that the third coin is a nickel?

10. If a student knows 75% of the material in a course, and a 100 question multiple choice test with five choices per question covers the material in a balanced way, what is the student's probability of getting a right answer to a given question, given that the student guesses at the answer to each question whose answer he or she does not know?

11. Suppose E and F are events with $E \cap F = \emptyset$. Describe when E and F are independent and explain why.

12. What is the probability that in a family consisting of a mother, father and two children of different ages, that the family has two girls, given that one of the children is a girl? What is the probability that the children are both boys, given that the older child is a boy?

5.4 Random Variables

What are Random Variables?

A **random variable** for an experiment with a sample space S is a function that assigns a number to each element of S. Typically instead of using f to stand for such a function we use X (at first, a random variable was conceived of as a variable related to an experiment, explaining the use of X, but it is very helpful in understanding the mathematics to realize it actually is a function on the sample space).

For example, if we consider the process of flipping a coin n times, we have the set of all sequences of n Hs and Ts as our sample space. The "number of heads" random variable takes a sequence and tells us how many heads are in that sequence. Somebody might say "Let X be the number of heads in 5 flips of a coin." In that case $X(HTHHT) = 3$ while $X(THTHT) = 2$. It may be rather jarring to see X used to stand for a function, but it is the notation most people use.

For a sequence of hashes of n keys into a table with k locations, we might have a random variable X_i which is the number of keys that are hashed to location i of the table, or a random variable X that counts the number of collisions (hashes to a location that already has at least one key). For an n question test on which each answer is either right or wrong (a short answer, True-False or multiple choice test for example) we could have a random variable that gives the number of right answers in a particular sequence of answers to the test. For a meal at a restaurant we might have a random variable that gives the price of any particular sequence of choices of menu items.

Exercise 5.4-1 Give several random variables that might be of interest to a doctor whose sample space is her patients.

Exercise 5.4-2 If you flip a coin six times, how many heads do you expect?

A doctor might be interested in patients' ages, weights, temperatures, blood pressures, cholesterol levels, etc.

For Exercise 5.4-2, in six flips of a coin, it is natural to expect three heads. We might argue that if we average the number of heads over all possible outcomes, the average should be half the number of flips. Since the probability of any given sequence equals that of any other, it is reasonable to say that this average is what we expect. Thus we would say we expect the number of heads to be half the number of flips. We will explore this more formally later.

Binomial Probabilities

When we study an independent trials process with two outcomes at each stage, it is traditional to refer to those outcomes as successes and failures. When we are flipping a coin, we are often interested in the number of heads. When we are analyzing student performance on a test, we are interested in the number of correct answers. When we are analyzing the outcomes in drug trials, we are interested in the number of trials where the drug was successful in treating the disease. This suggests a natural random variable associated with an independent trials process with two outcomes at each stage, namely the number of successes in n trials. We will analyze in general the probability of exactly k successes in n independent trials with probability p of success (and thus probability $1-p$ of failure) on each trial. It is standard to call such an independent trials process a *Bernoulli trials process.*

Exercise 5.4-3 Suppose we have 5 Bernoulli trials with probability p of success on each trial. What is the probability of success on the first three trials and failure on the last two? Failure on the first two trials and success on the last three? Success on trials 1, 3, and 5, and failure on the other two? Success on any particular three trials, and failure on the other two?

Since the probability of a sequence of outcomes is the product of the probabilities of the individual outcomes, the probability of any sequence of 3 successes and 2 failures is $p^3(1-p)^2$. More generally, in n Bernoulli trials, the probability of a given sequence of k successes and $n-k$ failures is $p^k(1-p)^{n-k}$. However this is not the probability of having k successes, because many different sequences could have k successes.

How many sequences of n successes and failures have exactly k successes? The number of ways to choose the k places out of n where the successes occur is $\binom{n}{k}$, so the number of sequences with k successes is $\binom{n}{k}$. This paragraph and the last together give us Theorem 5.7.

Theorem 5.7 *The probability of having exactly k successes in a sequence of n independent trials with two outcomes and probability p of success on each trial is*

$$P(\textit{exactly } k \textit{ successes}) = \binom{n}{k} p^k (1-p)^{n-k}$$

.

Proof: The proof follows from the two paragraphs preceding the theorem.■

Because of the connection between these probabilities and the binomial coefficients, the probabilities of Theorem 5.7 are called **binomial probabilities**, or the **binomial probability distribution**.

Exercise 5.4-4 A student takes a ten question objective test. Suppose that a student who knows 80% of the course material has probability .8 of success an any question, independently of how the student did on any other problem. What is the probability that this student earns a grade of 80 or better (out of 100)? What grade would you expect the student to get?

Exercise 5.4-5 Recall the primality testing algorithm from Section 2.4. Here we said that we could, by choosing a random number less than or equal to n, perform a test on n that, if n was not prime, would certify this fact with probability $1/2$. Suppose we perform 20 of these tests. It is reasonable to assume that each of these tests is independent of the rest of them. What is the probability that a non-prime number is certified to be non-prime?

Since a grade of 80 or better on a ten question test corresponds to 8, 9, or 10 successes in ten trials, in Exercise 5.4-4 we have

$$P(80 \text{ or better}) = \binom{10}{8}(.8)^8(.2)^2 + \binom{10}{9}(.8)^9(.2)^1 + (.8)^{10}.$$

Some work with a calculator gives us that this sum is approximately .678. The grade we would expect the student to get is 80.

In Exercise 5.4-5, we will first compute the probability that a non-prime number is not certified to be non-prime. If we think of success as when the number is certified non-prime and failure when it isn't, then we see that the only way to fail to certify a number is to have 20 failures. Using our formula we see that the probability that a non-prime number is not certified non-prime is just $\binom{20}{20}(.5)^{20} = 1/1048576$. Thus the chance of this happening is less than one in a million, and the chance of certifying the non-prime as non-prime is 1 minus this. Therefore the probability that a non-prime number will be certified non-prime is 1048575/1048576, which is more than .999999, so a non-prime number is almost sure to be certified non-prime.

A Taste of Generating Functions We note a nice connection between the probability of having exactly k successes and the binomial theorem. Consider, as an example, the polynomial $(H+T)^3$. Using the binomial theorem, we get that this is

$$(H+T)^3 = \binom{3}{0}H^3 + \binom{3}{1}H^2T + \binom{3}{2}HT^2 + \binom{3}{3}T^3.$$

We can interpret this as telling us that if we flip a coin three times, with outcomes heads or tails each time, then there are $\binom{3}{0} = 1$ way of getting 3 heads, $\binom{3}{2} = 3$ ways of getting two heads and one tail, $\binom{3}{1} = 3$ ways of getting one head and two tails and $\binom{3}{3} = 1$ way of getting 3 tails.

Similarly, if we replace H and T by px and $(1-p)y$ we would get the following:

$$(px + (1-p)y)^3 = \binom{3}{0}p^3x^3 + \binom{3}{1}p^2(1-p)x^2y + \binom{3}{2}p(1-p)^2xy^2 + \binom{3}{3}(1-p)^3y^3.$$

Generalizing this to n repeated trials where in each trial the probability of success is p, we see that by taking $(px + (1-p)y)^n$ we get

$$(px + (1-p)y)^n = \sum_{k=0}^{k} \binom{n}{k} p^k(1-p)^{n-k}x^ky^{n-k}.$$

Taking the coefficient of x^ky^{n-k} from this sum, we get exactly the result of Theorem 5.7. This connection is a simple case of a very powerful tool known as *generating functions*. We say that the polynomial $(px + (1-p)y)^n$ *generates* the binomial probabilities. In fact, we don't even need the y, because

$$(px + 1 - p)^n = \sum_{i=0}^{n} \binom{n}{i} p^i(1-p)^{n-i}x^i.$$

In general, the *generating function* for the sequence $a_0, a_1, a_2, \ldots, a_n$ is $\sum_{i=1}^{n} a_ix^i$, and the *generating function* for an infinite sequence $a_0, a_1, a_2, \ldots, a_n, \ldots$ is the infinite series $\sum_{i=1}^{\infty} a_ix^i$.

Expected Value

In Exercise 5.4-4 and Exercise 5.4-2 we asked about the value you would expect a random variable(in these cases, a test score and the number of heads in six flips of a coin) to have. We haven't yet defined what we mean by the value we expect, and yet it seems to make sense in the places we asked about it. If we say we expect 1 head if we flip a coin twice, we can explain our reasoning by taking an average. There are four outcomes, one with no heads, two with one head, and one with two heads, giving us an average of

$$\frac{0+1+1+2}{4} = 1.$$

Notice that using averages compels us to have some expected values that are impossible to achieve. For example in three flips of a coin the eight possibilities for the number of heads are 0, 1, 1, 1, 2, 2, 2, 3, giving us for our average

$$\frac{0+1+1+1+2+2+2+3}{8} = 1.5.$$

Exercise 5.4-6 An interpretation in games and gambling makes it clear that it makes sense to expect a random variable to have a value that is not one of the possible outcomes. Suppose that I proposed the following game. You pay me some money, and then you flip three coins. I will pay you one dollar for every head that comes up. Would you play this game if you had to pay me \$2.00? How about if you had to pay me \$1? How much do you think it should cost, in order for this game to be fair?

Since you expect to get 1.5 heads, you expect to make \$1.50. Therefore, it is reasonable to play this game as long as the cost is at most \$1.50.

Certainly averaging our variable over all elements of our sample space by adding up one result for each element of the sample space as we have done above is impractical even when we are talking about something as simple as ten flips of a coin. However we can ask how many times each possible number of heads arises, and then multiply the number of heads by the number of times it arises to get an average number of heads of

$$\frac{0\binom{10}{0} + 1\binom{10}{1} + 2\binom{10}{2} + \cdots + 9\binom{10}{9} + 10\binom{10}{10}}{1024} = \frac{\sum_{i=0}^{10} i\binom{10}{i}}{1024}. \tag{5.22}$$

Thus we wonder whether we have seen a formula for $\sum_{i=0}^{n} i\binom{n}{i}$. Perhaps we have, but in any case the binomial theorem and a bit of calculus or a proof by induction show that

$$\sum_{i=0}^{n} i\binom{n}{i} = 2^{n-1}n,$$

giving us $512 \cdot 10/1024 = 5$ for the fraction in Equation 5.22. If you are asking "Does it have to be that hard?" then good for you. Once we know a bit about the theory of expected values of random variables, computations like this will be replaced by far simpler ones.

Besides the nasty computations that a simple question lead us to, the average value of a random variable on a sample space need not have anything to do with the result we expect. For instance if we replace heads and tails with right and wrong, we get the sample space of possible results that a student will get when taking a ten question test with probability .9 of getting the right answer on any one question. Thus if we compute the average number of right answers in all the possible patterns of test results we get an average of 5 right answers. This is not the number of right answers we expect because averaging has nothing to do with the underlying process that gave us our probability! If we analyze the ten coin flips a bit more carefully, we can resolve this disconnection. We can rewrite Equation 5.22 as

$$0\frac{\binom{10}{0}}{1024} + 1\frac{\binom{10}{1}}{1024} + 2\frac{\binom{10}{2}}{1024} + \cdots + 9\frac{\binom{10}{9}}{1024} + 10\frac{\binom{10}{10}}{1024} = \sum_{i=0}^{10} i\frac{\binom{10}{i}}{1024}. \tag{5.23}$$

In Equation 5.23 we see we can compute the average number of heads by multiplying each value of our "number of heads" random variable by the probability that we have that value for our random variable, and then adding the results. This gives us a "weighted average" of the values of our random variable, each value weighted by its probability. Because the idea of weighting a random variable by its probability comes up so much in Probability Theory, there is a special notation that has developed to use this weight in equations. We use $P(X = x_i)$ to stand for the probability that the random variable X equals the value x_i. We call the function that assigns $P(x_i)$ to the event $P(X = x_i)$ the *distribution function* of the random variable X. Thus, for example, the binomial probability distribution is the distribution function for the "number of successes" random variable in Bernoulli trials.

We define the **expected value** or **expectation** of a random variable X whose values are the set $\{x_1, x_2, \ldots x_k\}$ to be

$$E(X) = \sum_{i=1}^{k} x_i P(X = x_i).$$

Then for someone taking a ten-question test with probability .9 of getting the correct answer on each question, the expected number of right answers is

$$\sum_{i=0}^{10} i\binom{10}{i}(.9)^i(.1)^{10-i}.$$

In the end of section exercises we will show a technique (that could be considered an application of generating functions) that allows us to compute this sum directly by using the binomial theorem and calculus. We now proceed to develop a less direct but easier way to compute this and many other expected values.

Exercise 5.4-7 Show that if a random variable X is defined on a sample space S (you may assume X has values x_1, x_2, $\ldots x_k$ as above) then the expected value of X is given by

$$E(X) = \sum_{s:s\in S} X(s)P(s).$$

(In words, we take each member of the sample space, compute its probability, multiply the probability by the value of the random variable and add the results.)

In Exercise 5.4-7 we asked for a proof of a fundamental lemma

Lemma 5.8 *If a random variable X is defined on a (finite) sample space S, then its expected value is given by*

$$E(X) = \sum_{s:s\in S} X(s)P(s).$$

Proof: Assume that the values of the random variable are x_1, x_2, $\ldots x_k$. Let F_i stand for the event that the value of X is x_i, so that $P(F_i) = P(X = x_i)$. Then, in the sum on the right-hand side of the equation in the statement of the lemma, we can take the items in the sample space, group them together into the events F_i and and rework the sum into the definition of expectation, as follows:

$$\begin{aligned}
\sum_{s:s\in S} X(s)P(s) &= \sum_{i=1}^{k} \sum_{s:s\in F_i} X(s)P(s) \\
&= \sum_{i=1}^{k} \sum_{s:s\in F_i} x_i P(s) \\
&= \sum_{i=1}^{k} x_i \sum_{s:s\in F_i} P(s) \\
&= \sum_{i=1}^{k} x_i P(F_i) \\
&= \sum_{i=1}^{k} x_i P(X = x_i) = E(X).
\end{aligned}$$

■

The proof of the lemma need not be so formal and symbolic as what we wrote; in English, it simply says that when we compute the sum in the Lemma, we can group together all elements of the sample space that have X-value x_i and add up their probabilities; this gives us $x_i P(x_i)$, which leads us to the definition of the expected value of X.

Expected Values of Sums and Numerical Multiples

Another important point about expected value follows naturally from what we think about when we use the word "expect" in English. If a paper grader expects to earn ten dollars grading papers today and expects to earn twenty dollars grading papers tomorrow, then she expects to earn thirty dollars grading papers in these two days. We could use X_1 to stand for the amount of money she makes grading papers today and X_2 to stand for the amount of money she makes grading papers tomorrow, so we are saying

$$E(X_1 + X_2) = E(X_1) + E(X_2).$$

This formula holds for any sum of a pair of random variables, and more generally for any sum of random variables on the same sample space.

Theorem 5.9 *Suppose X and Y are random variables on the (finite) sample space S. Then*

$$E(X + Y) = E(X) + E(Y).$$

Proof: From Lemma 5.8 we may write

$$E(X+Y) = \sum_{s:s\in S}(X(s)+Y(s))P(s) = \sum_{s:s\in S} X(s)P(s) + \sum_{s:s\in S} Y(s)P(s) = E(X)+E(Y).$$

■

If we double the credit we give for each question on a test, we would expect students' scores to double. Thus our next theorem should be no surprise. In it we use the notation cX for the random variable we get from X by multiplying all its values by the number c.

Theorem 5.10 *Suppose X is a random variable on a sample space S. Then for any number c, $E(cX) = cE(X)$.*

Proof: Left as a problem.■

Theorems 5.9 and 5.10 are very useful in proving facts about random variables. Taken together, they are typically called *linearity of expectation*. (The idea that the expectation of a sum is the same as the sum of expectations is called the *additivity of expectation*.) The idea of linearity will often allow us to work with expectations much more easily than if we had to work with the underlying probabilities.

For example, on one flip of a coin, our expected number of heads is .5. Suppose we flip a coin n times and let X_i be the number of heads we see on flip i, so that X_i is either 0 or 1. (For example in five flips of a coin, $X_2(HTHHT) = 0$ while $X_3(HTHHT) = 1$.) Then X, the total number of heads in n flips is given by

$$X = X_1 + X_2 + \cdots X_n, \tag{5.24}$$

the sum of the number of heads on the first flip, the number on the second, and so on through the number of heads on the last flip. But the expected value of each X_i is .5. We can take the expectation of both sides of Equation 5.24 and apply Lemma 5.9 repeatedly (or use induction) to get that

$$\begin{aligned} E(X) &= E(X_1 + X_2 + \cdots + X_n) \\ &= E(X_1) + E(X_2) + \cdots + E(X_n) \\ &= .5 + .5 + \cdots + .5 \\ &= .5n \end{aligned}$$

Thus in n flips of a coin, the expected number of heads is $.5n$. Compare the ease of this method with the effort needed earlier to deal with the expected number of heads in ten flips! Dealing with probability .9 or, in general with probability p poses no problem.

Exercise 5.4-8 Use the additivity of expectation to determine the expected number of correct answers a student will get on an n question "fill in the blanks" test if he or she knows 90% of the material in the course and the questions on the test are an accurate and uniform sampling of the material in the course.

In Exercise 5.4-8, since the questions sample the material in the course accurately, the most natural probability for us to assign to the event that the student gets a correct answer on a given question is .9. We can let X_i be the number of correct answers on question i (that is, either 1 or 0 depending on whether or not the student gets the correct answer). Then the expected number of right answers is the expected value of the sum of the variables X_i. From Theorem 5.9 see that in n trials with probability .9 of success, we expect to have $.9n$ successes. This gives that the expected number of right answers on a ten question test with probability .9 of getting each question right is 9, as we expected. This is a special case of our next theorem, which is proved by the same kind of computation.

Theorem 5.11 *In a Bernoulli trials process, in which each experiment has two outcomes and probability p of success, the expected number of successes is np.*

Proof: Let X_i be the number of successes in the ith of n independent trials. The expected number of successes on the ith trial (i.e. the expected value of X_i) is, by definition,

$$p \cdot 1 + (1-p) \cdot 0 = p.$$

The number of successes X in all n trials is the sum of the random variables X_i. Then by Theorem 5.9 the expected number of successes in n independent trials is the sum of the expected values of the n random variables X_i and this sum is np.■

The Number of Trials until the First Success

Exercise 5.4-9 How many times do you expect to have to flip a coin until you first see a head? Why? How many times to you expect to have to roll two dice until you see a sum of seven? Why?

Our intuition suggests that we should have to flip a coin twice to see a head. However we could conceivably flip a coin forever without seeing a head, so should we really expect to see a head in two flips? The probability of getting a seven on two dice is 1/6. Does that mean we should expect to have to roll the dice six times before we see a seven?

In order to analyze this kind of question we have to realize that we are stepping out of the realm of independent trials processes on finite sample spaces. We will consider the process of repeating independent trials with probability p of success until we have a success and then stopping. Now the possible outcomes of our multistage process are the infinite set

$$\{S, FS, FFS, \ldots, F^iS, \ldots\},$$

in which we have used the notation F^iS to stand for the sequence of i failures followed by a success. Since we have an infinite sequence of outcomes, it makes sense to think about whether we can assign an infinite sequence of probability weights to its members so that the resulting sequence of probabilities adds to one. If so, then all our definitions make sense, and in fact the proofs of all our theorems remain valid.[5] There is only one way to assign weights that is consistent with our knowledge of (finite) independent trials processes, namely

$$P(S) = p, \quad P(FS) = (1-p)p, \quad \ldots, \quad P(F^iS) = (1-p)^ip, \quad \ldots.$$

[5]for those who are familiar with the concept of convergence for infinite sums (i.e. infinite series), it is worth noting that it is the fact that probability weights cannot be negative and must add to one that makes all the sums we need to deal with for all the theorems we have proved so far converge. That doesn't mean all sums we might want to deal with will converge; some random variables defined on the sample space we have described will have infinite expected value. However those we need to deal with for the expected number of trials until success do converge.

Thus we have to hope these weights add to one; in fact their sum is

$$\sum_{i=0}^{\infty}(1-p)^i p = p\sum_{i=0}^{\infty}(1-p)^i = p\frac{1}{1-(1-p)} = \frac{p}{p} = 1.$$

Therefore we have a legitimate assignment of probabilities and the set of sequences

$$\{F, FS, FFS, FFFS, \ldots, F^iS, \ldots\}$$

is a sample space with these probability weights. This probability distribution, $P(F^iS) = (1-p)^i p$, is called a *geometric* distribution because of the geometric series we used in proving the probabilities sum to 1.

Theorem 5.12 *Suppose we have a sequence of trials in which each trial has two outcomes, success and failure, and where at each step the probability of success is p. Then the expected number of trials until the first success is $1/p$.*

Proof:

We consider the random variable X which is i if the first success is on trial i. (In other words, $X(F^{i-1}S)$ is i.) The probability that the first success is on trial i is $(1-p)^{i-1}p$, since in order for this to happen there must be $i-1$ failures followed by 1 success. The expected number of trials is the expected value of X, which is, by the definition of expected value and the previous two sentences,

$$\begin{aligned}
E[\text{number of trials}] &= \sum_{i=0}^{\infty} p(1-p)^{i-1}i \\
&= p\sum_{i=0}^{\infty}(1-p)^{i-1}i \\
&= \frac{p}{1-p}\sum_{i=0}^{\infty}(1-p)^i i \\
&= \frac{p}{1-p}\frac{1-p}{p^2} \\
&= \frac{1}{p}
\end{aligned}$$

To go from the third to the fourth line we used the fact that

$$\sum_{j=0}^{\infty} jx^j = \frac{x}{(1-x)^2}, \tag{5.25}$$

true for x with absolute value less than one. We proved a finite version of this equation as Theorem 4.6; the infinite version is even easier to prove. ■

Applying this theorem, we see that the expected number of times you need to flip a coin until you get heads is 2, and the expected number of times you need to roll two dice until you get a seven is 6.

Important Concepts, Formulas, and Theorems

1. *Random Variable.* A *random variable* for an experiment with a sample space S is a function that assigns a number to each element of S.

2. Bernoulli Trials Process. An independent trials process with two outcomes, success and failure, at each stage and probability p of success and $1-p$ of failure at each stage is called a *Bernoulli trials process.*

3. Probability of a Sequence of Bernoulli Trials. In n Bernoulli trials with probability p of success, the probability of a given sequence of k successes and $n-k$ failures is $p^k(1-p)^{n-k}$.

4. *The Probability of k Successes in n Bernoulli Trials* The probability of having exactly k successes in a sequence of n independent trials with two outcomes and probability p of success on each trial is
$$P(\text{exactly } k \text{ successes}) = \binom{n}{k} p^k (1-p)^{n-k}$$
.

5. Binomial Probability Distribution. The probabilities of of k successes in n Bernoulli trials, $\binom{n}{k}p^k(1-p)^{n-k}$, are called *binomial probabilities*, or the *binomial probability distribution.*

6. *Generating Function.* The *generating function* for the sequence $a_0, a_1, a_2, \ldots, a_n$ is $\sum_{i=1}^{n} a_i x^i$, and the *generating function* for an infinite sequence $a_0, a_1, a_2, \ldots, a_n, \ldots$ is the infinite series $\sum_{i=1}^{\infty} a_i x^i$. The polynomial $(px+1-p)^n$ is the generating function for the binomial probabilities for n Bernoulli trials with probability p of success.

7. *Distribution Function.* We call the function that assigns $P(x_i)$ to the event $P(X = x_i)$ the *distribution function* of the random variable X.

8. *Expected Value.* We define the *expected value* or *expectation* of a random variable X whose values are the set $\{x_1, x_2, \ldots x_k\}$ to be
$$E(X) = \sum_{i=1}^{k} x_i P(X = x_i).$$

9. *Another Formula for Expected Values.* If a random variable X is defined on a (finite) sample space S, then its expected value is given by
$$E(X) = \sum_{s:s\in S} X(s)P(s).$$

10. *Expected Value of a Sum.* Suppose X and Y are random variables on the (finite) sample space S. Then
$$E(X+Y) = E(X) + E(Y).$$
This is called the *additivity of expectation.*

11. *Expected Value of a Numerical Multiple.* Suppose X is a random variable on a sample space S. Then for any number c, $E(cX) = cE(X)$. This result and the additivity of expectation together are called the *linearity of expectation.*

12. *Expected Number of Successes in Bernoulli Trials.* In a Bernoulli trials process, in which each experiment has two outcomes and probability p of success, the expected number of successes is np.

13. *Expected Number of Trials Until Success.* Suppose we have a sequence of trials in which each trial has two outcomes, success and failure, and where at each step the probability of success is p. Then the expected number of trials until the first success is $1/p$.

Problems

1. Give several random variables that might be of interest to someone rolling five dice (as one does, for example, in the game Yatzee).

2. Suppose I offer to play the following game with you if you will pay me some money. You roll a die, and I give you a dollar for each dot that is on top. What is the maximum amount of money a rational person might be willing to pay me in order to play this game?

3. How many sixes do we expect to see on top if we roll 24 dice?

4. What is the expected sum of the tops of n dice when we roll them?

5. In an independent trials process consisting of six trials with probability p of success, what is the probability that the first three trials are successes and the last three are failures? The probability that the last three trials are successes and the first three are failures? The probability that trials 1, 3, and 5 are successes and trials 2, 4, and 6 are failures? What is the probability of three successes and three failures?

6. What is the probability of exactly eight heads in ten flips of a coin? Of eight or more heads?

7. How many times do you expect to have to role a die until you see a six on the top face?

8. Assuming that the process of answering the questions on a five-question quiz is an independent trials process and that a student has a probability of .8 of answering any given question correctly, what is the probability of a sequence of four correct answers and one incorrect answer? What is the probability that a student answers exactly four questions correctly?

9. What is the expected value of the constant random variable X that has $X(s) = c$ for every member s of the sample space? We frequently just use c to stand for this random variable, and thus this question is asking for $E(c)$.

10. Someone is taking a true-false test and guessing when they don't know the answer. We are going to compute a score by subtracting a percentage of the number of incorrect answers from the number of correct answers. When we convert this "corrected score" to a percentage score we want its expected value to be the percentage of the material being tested that the test-taker knows. How can we do this?

11. Do Problem 10 of this section for the case that someone is taking a multiple choice test with five choices for each answer and guesses randomly when they don't know the answer.

12. Suppose we have ten independent trials with three outcomes called good, bad, and indifferent, with probabilities p, q, and r, respectively. What is the probability of three goods, two bads, and five indifferents? In n independent trials with three outcomes A, B, and C, with probabilities p, q, and r, what is the probability of i As, j Bs, and k Cs? (In this problem we assume $p+q+r=1$ and $i+j+k=n$.)

13. In as many ways as you can, prove that
$$\sum_{i=0}^{n} i\binom{n}{i} = 2^{n-1}n.$$

14. Prove Theorem 5.10.

15. Two nickels, two dimes, and two quarters are in a cup. We draw three coins, one after the other, without replacement. What is the expected amount of money we draw on the first draw? On the second draw? What is the expected value of the total amount of money we draw? Does this expected value change if we draw the three coins all together?

16. In this exercise we will evaluate the sum
$$\sum_{i=0}^{10} i\binom{10}{i}(.9)^i(.1)^{10-i}$$
that arose in computing the expected number of right answers a person would have on a ten question test with probability .9 of answering each question correctly. First, use the binomial theorem and calculus to show that
$$10(.1+x)^9 = \sum_{i=0}^{10} i\binom{10}{i}(.1)^{10-i}x^{i-1}$$
Substituting in $x = .9$ gives us almost the sum we want on the right hand side of the equation, except that in every term of the sum the power on .9 is one too small. Use some simple algebra to fix this and then explain why the expected number of right answers is 9.

17. Give an example of two random variables X and Y such that $E(XY) \neq E(X)E(Y)$. Here XY is the random variable with $(XY)(s) = X(s)Y(s)$.

18. Prove that if X and Y are independent in the sense that the event that $X = x$ and the event that $Y = y$ are independent for each pair of values x of X and y of Y, then $E(XY) = E(X)E(Y)$. See Exercise 5-17 for a definition of XY.

19. Use calculus and the sum of a geometric series to show that
$$\sum_{j=0}^{\infty} jx^j = \frac{x}{(1-x)^2}$$
as in Equation 5.25.

20. Give an example of a random variable on the sample space $\{S, FS, FFS, \ldots, F^iS, \ldots\}$ with an infinite expected value.

5.5 Probability Calculations in Hashing

We can use our knowledge of probability and expected values to analyze a number of interesting aspects of hashing including:

1. expected number of items per location,
2. expected time for a search,
3. expected number of collisions,
4. expected number of empty locations,
5. expected time until all locations have at least one item,
6. expected maximum number of items per location.

Expected Number of Items per Location

Exercise 5.5-1 We are going to compute the expected number of items that hash to any particular location in a hash table. Our model of hashing n items into a table of size k allows us to think of the process as n independent trials, each with k possible outcomes (the k locations in the table). On each trial we hash another key into the table. If we hash n items into a table with k locations, what is the probability that any one item hashes into location 1? Let X_i be the random variable that counts the number of items that hash to location 1 in trial i (so that X_i is either 0 or 1). What is the expected value of X_i? Let X be the random variable $X_1 + X_2 + \cdots + X_n$. What is the expected value of X? What is the expected number of items that hash to location 1? Was the fact that we were talking about location 1 special in any way? That is, does the same expected value apply to every location?

Exercise 5.5-2 Again we are hashing n items into k locations. Our model of hashing is that of Exercise 5.5-1. What is the probability that a location is empty? What is the expected number of empty locations? Suppose we now hash n items into the same number n of locations. What limit does the expected fraction of empty places approach as n gets large?

In Exercise 5.5-1, the probability that any one item hashes into location 1 is $1/k$, because all k locations are equally likely. The expected value of X_i is then $1/k$. The expected value of X is then n/k, the sum of n terms each equal to $1/k$. Of course the same expected value applies to any location. Thus we have proved the following theorem.

Theorem 5.13 *In hashing n items into a hash table of size k, the expected number of items that hash to any one location is n/k.*

Expected Number of Empty Locations

In Exercise 5.5-2 the probability that position i will be empty after we hash 1 item into the table will be $1 - \frac{1}{k}$. (Why?) In fact, we can think of our process as an independent trials process with two outcomes: the key hashes to slot i or it doesn't. From this point of view, it is clear that the probability of nothing hashing to slot i in n trials is $(1 - \frac{1}{k})^n$. Now consider the original sample space again and let X_i be 1 if slot i is empty for a given sequence of hashes or 0 if it is not. Then the number of empty slots for a given sequence of hashes is $X_1 + X_2 + \cdots + X_k$ evaluated at that sequence. Therefore, the expected number of empty slots is, by Theorem 5.9, $k(1 - \frac{1}{k})^n$. Thus we have proved another nice theorem about hashing.

Theorem 5.14 *In hashing n items into a hash table with k locations, the expected number of empty locations is $k(1 - \frac{1}{k})^n$.*

Proof: Given above.■

If we have the same number of slots as places, the expected number of empty slots is $n(1-\frac{1}{n})^n$, so the expected fraction of empty slots is $(1 - \frac{1}{n})^n$. What does this fraction approach as n grows? You may recall that $\lim_{n\to\infty}(1 + \frac{1}{n})^n$ is e, the base for the natural logarithm. In the problems at the end of the section, we show you how to derive from this that $\lim_{n\to\infty}(1 - \frac{1}{n})^n$ is e^{-1}. Thus for a reasonably large hash table, if we hash in as many items as we have slots, we expect a fraction $1/e$ of those slots to remain empty. In other words, we expect n/e empty slots. On the other hand, we expect $\frac{n}{n}$ items per location, which suggests that we should expect each slot to have an item and therefore expect to have no empty locations. Is something wrong? No, but we simply have to accept that our expectations about expectation just don't always hold true. What went wrong in that apparent contradiction is that our definition of expected value doesn't imply that if we have an expectation of one key per location then every location must have a key, but only that empty locations have to be balanced out by locations with more than one key. When we want to make a statement about expected values, we must use either our definitions or theorems to back it up. This is another example of why we have to back up intuition about probability with careful analysis.

Expected Number of Collisions

We say that we have a *collision* when we hash an item to a location that already contains an item. How can we compute the expected number of collisions? The number of collisions will be the number n of keys hashed minus the number of occupied locations because each occupied location will contain one key that will not have collided in the process of being hashed. Thus, by Theorems 5.9 and 5.10,

$$E(\text{collisions}) = n - E(\text{occupied locations}) = n - k + E(\text{empty locations}) \tag{5.26}$$

where the last equality follows because the expected number of occupied locations is k minus the expected number of unoccupied locations. This gives us yet another theorem.

Theorem 5.15 *In hashing n items into a hash table with k locations, the expected number of collisions is $n - k + k(1 - \frac{1}{k})^n$.*

Proof: We have already shown in Theorem 5.14 that the expected number of empty locations is $k(1-\frac{1}{k})^n$. Substituting this into Equation 5.26 gives our formula. ■

Exercise 5.5-3 In real applications, it is often the case that the hash table size is not fixed in advance, since you don't know, in advance, how many items you will insert. The most common heuristic for dealing with this is to start k, the hash table size, at some reasonably small value, and then when n, the number of items, gets to be greater than $2k$, you double the hash table size. In this exercise we propose a different idea. Suppose you waited until every single slot in the hash table had at least one item in it, and then you increased the table size. What is the expected number of items that will be in the table when you increase the size? In other words, how many items do you expect to insert into a hash table in order to ensure that every slot has at least one item? (Hint: Let X_i be the number of items added between the time that there are $i-1$ occupied slots for the first time and the first time that there are i occupied slots.)

For Exercise 5.5-3, the key is to let X_i be the number of items added between the time that there are $i-1$ full slots for the first time and i full slots for the first time. Let's think about this random variable. $E(X_1) = 1$, since after one insertion there is one full slot. In fact X_1 itself is equal to 1.

To compute the expected value of X_2, we note that X_2 can take on any value greater than 1. In fact if we think about it, what we have here (until we actually hash an item to a new slot) is an independent trials process with two outcomes, with success meaning our item hashes to an unused slot. X_2 counts the number of trials until the first success. The probability of success is $(k-1)/k$. In asking for the expected value of X_2, we are asking for expected number of steps until the first success. Thus we can apply Lemma 5.12 to get that it is $k/(k-1)$.

Continuing, X_3 similarly counts the number of steps in an independent trials process (with two outcomes) that stops at the first success and has probability of success $(k-2)/k$. Thus the expected number of steps until the first success is $k/(k-2)$.

In general, we have that X_i counts the number of trials until success in an independent trials process with probability of success $(k-i+1)/k$ and thus the expected number of steps until the first success is $k/(k-i+1)$, which is the expected value of X_i.

The total time until all slots are full is just $X = X_1 + \cdots + X_k$. Taking expectations and using Lemma 5.12 we get

$$\begin{aligned}
E(X) &= \sum_{j=1}^{k} E(X_j) \\
&= \sum_{j=1}^{k} \frac{k}{k-j+1} \\
&= k\sum_{j=1}^{k} \frac{1}{k-j+1} \\
&= k\sum_{k-j+1=1}^{k} \frac{1}{k-j+1}
\end{aligned}$$

$$= \quad k\sum_{i=1}^{k}\frac{1}{i},$$

where the last line follows just by switching the variable of the summation, that is, letting $k-j+1=i$ and summing over i.[6] Now the quantity $\sum_{i=1}^{k}\frac{1}{i}$ is known as a *harmonic number*, and is sometimes denoted by H_k. It is well known (and you can see why in the problems at the end of the section) that $\sum_{i=1}^{k}\frac{1}{i}=\Theta(\log k)$, and more precisely

$$\frac{1}{4}+\ln k \le H_k \le 1+\ln k, \tag{5.27}$$

and in fact,

$$\frac{1}{2}+\ln k \le H_k \le 1+\ln k, \tag{5.28}$$

when k is large enough. As n gets large, $H_n-\ln n$ approaches a limit called *Euler's constant*; Euler's constant is about .58. Equation 5.27 gives us that $E(X)=O(k\log k)$.

Theorem 5.16 *The expected number of items needed to fill all slots of a hash table of size k is between $k\ln k+\frac{1}{2}k$ and $k\ln k+k$.*

Proof: Given above. ■

So in order to fill every slot in a hash table of size k, we need to hash roughly $k\ln k$ items. This problem is sometimes called the *coupon collectors problem*.

The remainder of this section is devoted to proving that if we hash n items into a hash table with n slots, then the expected number of items per slot is $O(\log n/\log\log n)$. It should be no surpise that a result of this form requires a somewhat complex proof. The remainder of this section can be skipped without losss of continuity.

Expected maximum number of elements in a slot of a hash table (Optional)

In a hash table, the time to find an item is related to the number of items in the slot where you are looking. Thus an interesting quantity is the expected maximum length of the list of items in a slot in a hash table. This quantity is more complicated than many of the others we have been computing, and hence we will only try to upper bound it, rather than compute it exactly. In doing so, we will introduce a few upper bounds and techniques that appear frequently and are useful in many areas of mathematics and computer science. We will be able to prove that if we hash n items into a hash table of size n, the expected length of the longest list is $O(\log n/\log\log n)$. One can also prove, although we won't do it here, that with high probability, there will be some list with $\Omega(\log n/\log\log n)$ items in it, so our bound is, up to constant factors, the best possible.

Before we start, we give some useful upper bounds. The first allows us to bound terms that look like $(1+\frac{1}{x})^x$, for any positive x, by e.

Lemma 5.17 *For all $x>0$, $(1+\frac{1}{x})^x\le e$.*

[6] Note that $k-j+1$ runs from k to 1 as j runs from 1 to k, so we are describing exactly the same sum.

Proof: $\lim_{x\to\infty}(1+\frac{1}{x})^x = e$, and $(1+\frac{1}{x})^x$ has positive first derivative. ■

Second, we will use an approximation called Stirling's formula,

$$x! = \left(\frac{x}{e}\right)^x \sqrt{2\pi x}(1+\Theta(1/n)),$$

which tells us, roughly, that $(x/e)^x$ is a good approximation for $x!$. Moreover the constant in the $\Theta(1/n)$ term is extremely small, so for our purposes we will just say that

$$x! = \left(\frac{x}{e}\right)^x \sqrt{2\pi x}.$$

(We use this equality only in our proof of Lemma 5.18. You will see in that Lemma that we make the statement that $\sqrt{2\pi} > 1$. In fact, $\sqrt{2\pi} > 2$, and this is more than enough to make up for any lack of accuracy in our approximation.) Using Stirling's formula, we can get a bound on $\binom{n}{t}$,

Lemma 5.18 *For $n > t > 0$,*

$$\binom{n}{t} \le \frac{n^n}{t^t(n-t)^{n-t}}.$$

Proof:

$$\begin{aligned}
\binom{n}{t} &= \frac{n!}{t!(n-t)!} && (5.29)\\
&= \frac{(n/e)^n\sqrt{2\pi n}}{(t/e)^t\sqrt{2\pi t}((n-t)/e)^{n-t}\sqrt{2\pi(n-t)}} && (5.30)\\
&= \frac{n^n\sqrt{n}}{t^t(n-t)^{n-t}\sqrt{2\pi}\sqrt{t(n-t)}} && (5.31)
\end{aligned}$$

Now if $1 < t < n-1$, we have $t(n-t) \ge n$, so that $\sqrt{t(n-t)} \ge \sqrt{n}$. Further $\sqrt{2\pi} > 1$. We can use these facts to upper bound the quantity marked 5.31 by

$$\frac{n^n}{t^t(n-t)^{n-t}}.$$

When $t = 1$ or $t = n-1$, the inequality in the statement of the lemma is $n \le n^n/(n-1)^{n-1}$ which is true since $n-1 < n$. ■

We are now ready to attack the problem at hand, the expected value of the maximum list size. Let's start with a related quantity that we already know how to compute. Let H_{it} be the event that t keys hash to slot i. $P(H_{it})$ is just the probability of t successes in an independent trials process with success probability $1/n$, so

$$P(H_{it}) = \binom{n}{t}\left(\frac{1}{n}\right)^t\left(1-\frac{1}{n}\right)^{n-t}. \tag{5.32}$$

Now we relate this known quantity to the probability of the event M_t that the maximum list size is t.

Lemma 5.19 *Let M_t be the event that t is the maximum list size in hashing n items into a hash table of size n. Let H_{1t} be the event that t keys hash to position 1. Then*

$$P(M_t) \leq nP(H_{1t})$$

Proof: We begin by letting M_{it} be the event that the maximum list size is t and this list appears in slot i. Observe that that since M_{it} is a subset of H_{it},

$$P(M_{it}) \leq P(H_{it}). \tag{5.33}$$

We know that, by definition,

$$M_t = M_{1t} \cup \cdots \cup M_{nt},$$

and so

$$P(M_t) = P(M_{1t} \cup \cdots \cup M_{nt}).$$

Therefore, since the sum of the probabilities of the individual events must be at least as large as the probability of the union,

$$P(M_t) \leq P(M_{1t}) + P(M_{2t}) + \cdots + P(M_{nt}). \tag{5.34}$$

(Recall that we introduced the Principle of Inclusion and Exclusion because the right hand side overestimated the probability of the union. Note that the inequality in Equation 5.34 holds for any union, not just this one: it is sometimes called *Boole's inequality*.)

In this case, for any i and j, $P(M_{it}) = P(M_{jt})$, since there is no reason for slot i to be more likely than slot j to be the maximum. We can therefore write that

$$P(M_t) = nP(M_{1t}) \leq nP(H_{1t}).$$

■

Now we can use Equation 5.32 for $P(H_{1t})$ and then apply Lemma 5.18 to get that

$$\begin{aligned} P(H_{1t}) &= \binom{n}{t}\left(\frac{1}{n}\right)^t\left(1-\frac{1}{n}\right)^{n-t} \\ &\leq \frac{n^n}{t^t(n-t)^{n-t}}\left(\frac{1}{n}\right)^t\left(1-\frac{1}{n}\right)^{n-t}. \end{aligned}$$

We continue, using algebra, the fact that $(1-\frac{1}{n})^{n-t} \leq 1$ and Lemma 5.17 to get

$$\begin{aligned} &\leq \frac{n^n}{t^t(n-t)^{n-t}n^t} \\ &= \frac{n^{n-t}}{t^t(n-t)^{n-t}} \\ &= \left(\frac{n}{n-t}\right)^{n-t}\frac{1}{t^t} \\ &= \left(1+\frac{t}{n-t}\right)^{n-t}\frac{1}{t^t} \\ &= \left(\left(1+\frac{t}{n-t}\right)^{\frac{n-t}{t}}\right)^t\frac{1}{t^t} \\ &\leq \frac{e^t}{t^t}. \end{aligned}$$

We have shown the following:

Lemma 5.20 *$P(M_t)$, the probability that the maximum list length is t, is at most ne^t/t^t.*

Proof: Our sequence of equations and inequalities above showed that $P(H_{1t}) \le \frac{e^t}{t^t}$. Multiplying by n and applying Lemma 5.19 gives our result.■

Now that we have a bound on $P(M_t)$, we can compute a bound on the expected length of the longest list, namely

$$\sum_{t=0}^{n} P(M_t)t.$$

However, if we think carefully about the bound in Lemma 5.20, we see that we have a problem. For example when $t = 1$, the lemma tells us that $P(M_1) \le ne$. This is vacuous, as we know that any probability is at most 1. We could make a stronger statement that $P(M_t) \le \max\{ne^t/t^t, 1\}$, but even this wouldn't be sufficient, since it would tell us things like $P(M_1) + P(M_2) \le 2$, which is also vacuous. All is not lost however. Our lemma causes this problem only when t is small. We will split the sum defining the expected value into two parts and bound the expectation for each part separately. The intuition is that when we restrict t to be small, then $\sum P(M_t)t$ is small because t is small (and over all t, $\sum P(M_t) \le 1$). When t gets larger, Lemma 5.20 tells us that $P(M_t)$ is very small and so the sum doesn't get big in that case either. We will choose a way to split the sum so that this second part of the sum is bounded by a constant. In particular we split the sum up by

$$\sum_{t=0}^{n} P(M_t)t \le \sum_{t=0}^{\lfloor 5\log n/\log\log n\rfloor} P(M_t)t + \sum_{t=\lceil 5\log n/\log\log n\rceil}^{n} P(M_t)t \tag{5.35}$$

For the sum over the smaller values of t, we just observe that in each term $t \le 5\log n/\log\log n$ so that

$$\begin{aligned} \sum_{t=0}^{5\log n/\log\log n} P(M_t)t &\le \sum_{t=0}^{5\log n/\log\log n} P(M_t) 5\log n/\log\log n && (5.36)\\ &= 5\log n/\log\log n \sum_{t=0}^{5\log n/\log\log n} P(M_t) && (5.37)\\ &\le 5\log n/\log\log n && (5.38) \end{aligned}$$

(Note that we are not using Lemma 5.20 here; only the fact that the probabilities of disjoint events cannot add to more than 1.) For the rightmost sum in Equation 5.35, we want to first compute an upper bound on $P(M_t)$ for $t = (5\log n/\log\log n)$. Using Lemma 5.20, and doing a bit of calculation we get that in this case $P(M_t) \le 1/n^2$. Since the bound on $P(M_t)$ from Lemma 5.20 decreases as t grows, and $t \le n$, we can bound the right sum by

$$\sum_{t=5\log n/\log\log n}^{n} P(M_t)t \le \sum_{t=5\log n/\log\log n}^{n} \frac{1}{n^2}n \le \sum_{t=5\log n/\log\log n}^{n} \frac{1}{n} \le 1. \tag{5.39}$$

Combining Equations 5.38 and 5.39 with 5.35 we get the desired result.

Theorem 5.21 *If we hash n items into a hash table of size n, the expected maximum list length is $O(\log n/\log\log n)$.*

The choice to break the sum into two pieces here—and especially the breakpoint we chose—may have seemed like magic. What is so special about $\log n / \log\log n$? Consider the bound on $P(M_t)$. If you asked what is the value of t for which the bound equals a certain value, say $1/n^2$, you get the equation $ne^t/t^t = n^{-2}$. If we try to solve the equation $ne^t/t^t = n^{-2}$ for t, we quickly see that we get a form that we do not know how to solve. (Try typing this into Mathematica or Maple, to see that it can't solve this equation either.) The equation we need to solve is somewhat similar to the simpler equation $t^t = n$. While this equation does not have a closed form solution, one can show that the t that satisfies this equation is roughly $c \log n / \log\log n$, for some constant c. This is why some multiple of $\log n / \log\log n$ made sense to try as the the magic value. For values much less than $\log n / \log\log n$ the bound provided on $P(M_t)$ is fairly large. Once we get past $\log n / \log\log n$, however, the bound on $P(M_t)$ starts to get significantly smaller. The factor of 5 was chosen by experimentation to make the second sum come out to be less than 1. We could have chosen any number between 4 and 5 to get the same result; or we could have chosen 4 and the second sum would have grown no faster than the first.

Important Concepts, Formulas, and Theorems

1. *Expected Number of Keys per Slot in Hash Table.* In hashing n items into a hash table of size k, the expected number of items that hash to any one location is n/k.

2. *Expected Number of Empty Slots in Hash Table.* In hashing n items into a hash table with k locations, the expected number of empty locations is $k(1 - \frac{1}{k})^n$.

3. *Collision in Hashing.* We say that we have a *collision* when we hash an item to a location that already contains an item.

4. *The Expected Number of Collisions in Hashing.* In hashing n items into a hash table with k locations, the expected number of collisions is $n - k + k(1 - \frac{1}{k})^n$.

5. *Harmonic Number.* The quantity $\sum_{i=1}^{k} \frac{1}{i}$ is known as a *harmonic number*, and is sometimes denoted by H_k. It is a fact that that $\sum_{i=1}^{k} \frac{1}{i} = \Theta(\log k)$, and more precisely

$$\frac{1}{2} + \ln k \le H_k \le 1 + \ln k.$$

6. *Euler's Constant.* As n gets large, $H_n - \ln n$ approaches a limit called *Euler's constant*; Euler's constant is about .58.

7. *Expected Number of Hashes until all Slots of a Hash Table are Occupied.* The expected number of items needed to fill all slots of a hash table of size k is between $k \ln k + \frac{1}{2}k$ and $k \ln k + k$.

8. *Expected Maximum Number of Keys per Slot.* If we hash n items into a hash table of size n, the expected maximum list length is $O(\log n / \log\log n)$.

9. *Stirling's Formula for $n!$. (Optional.)* $n!$ is approximately $\left(\frac{n}{e}\right)^n \sqrt{2\pi n}$.

Problems

1. A candy machine in a school has d different kinds of candy. Assume (for simplicity) that all these kinds of candy are equally popular and there is a large supply of each. Suppose that c children come to the machine and each purchases one package of candy. One of the kinds of candy is a Snackers bar. What is the probability that any given child purchases a Snackers bar? Let Y_i be the number of Snackers bars that child i purchases, so that Y_i is either 0 or 1. What is the expected value of Y_i? Let Y be the random variable $Y_1 + Y_2 + \cdots + Y_c$. What is the expected value of Y? What is the expected number of Snackers bars that is purchased? Does the same result apply to any of the varieties of candy?

2. Again as in the previous exercise, we have c children choosing from among ample supplies of d different kinds of candy, one package for each child, and all choices equally likely. What is the probability that a given variety of candy is chosen by no child? What is the expected number of kinds of candy chosen by no child? Suppose now that $c = d$. What happens to the expected number of kinds of candy chosen by no child?

3. How many children do we expect to have to observe buying candy until someone has bought a Snackers bar?

4. How many children to we expect to have to observe buying candy until each type of candy has been selected at least once?

5. If we have 20 kinds of candy, how many children have to buy candy in order for the probability to be at least one half that (at least) two children buy the same kind of candy?

6. What is the expected number of duplications among all the candy the children have selected?

7. Compute the values on the left-hand and right-hand side of the inequality in Lemma 5.18 for $n = 2$, $t = 0, 1, 2$ and for $n = 3$, $t = 0, 1, 2, 3$.

8. When we hash n items into k locations, what is the probability that all n items hash to different locations? What is the probability that the ith item is the first collision? What is the expected number of items we must hash until the first collision? Use a computer program or spreadsheet to compute the expected number of items hashed into a hash table until the first collision with $k = 20$ and with $k = 100$.

9. We have seen a number of occasions when our intuition about expected values or probability in general fails us. When we wrote down Equation 5.26 we said that the expected number of occupied locations is k minus the expected number of unoccupied locations. While this seems obvious, there is a short proof. Give the proof.

10. Write a computer program that prints out a table of values of the expected number of collisions with n keys hashed into a table with k locations for interesting values of n and k. Does this value vary much as n and k change?

11. Suppose you hash n items into a hash table of size k. It is natural to ask about the time it takes to find an item in the hash table. We can divide this into two cases, one when the item is not in the hash table (an unsuccessful search), and one when the item is in the hash table (a successful search). Consider first the unsuccessful search. Assume the keys hashing

to the same location are stored in a list with the most recent arrival at the beginning of the list. Use our expected list length to bound the expected time for an unsuccessful search. Next consider the successful search. Recall that when we insert items into a hash table, we typically insert them at the beginning of a list, and so the time for a successful search for item i should depend on how many entries were inserted after item i. Carefully compute the expected running time for a successful search. Assume that the item you are searching for is randomly chosen from among the items already in the table. (Hint: The unsuccessful search should take roughly twice as long as the successful one. Be sure to explain why this is the case.)

12. Suppose I hash $n \log n$ items into n buckets. What is the expected maximum number of items in a bucket?

13. The fact that $\lim_{n\to\infty}(1+\frac{1}{n})^n = e$ (where n varies over integers) is a consequence of the fact that $\lim_{h\to 0}(1+h)^{\frac{1}{h}} = e$ (where h varies over real numbers). Thus if h varies over negative real numbers, but approaches 0, the limit still exists and equals e. What does this tell you about $\lim_{n\to -\infty}(1+\frac{1}{n})^n$? Using this and rewriting $(1-\frac{1}{n})^n$ as $(1+\frac{1}{-n})^n$ show that

14. What is the expected number of empty slots when we hash $2k$ items into a hash table with k slots? What is the expected fraction of empty slots close to when k is reasonably large?

15. Using whatever methods you like (hand calculations or computer), give upper and/or lower bounds on the value of the x satisfying $x^x = n$.

16. Professor Max Weinberger decides that the method proposed for computing the maximum list size is much too complicated. He proposes the following solution. Let X_i be the size of list i. Then what we want to compute is $E(\max_i(X_i))$. Well

$$E(\max_i(X_i)) = \max_i(E(X_i)) = \max_i(1) = 1.$$

What is the flaw in his solution?

17. Prove as tight upper and lower bounds as you can on $\sum_{i=1}^{k}\frac{1}{i}$. For this purpose it is useful to remember the definition of the natural logarithm as an integral involving $1/x$ and to draw rectangles and other geometric figures above and below the curve.

18. Notice that $\ln n! = \sum_{i=1}^{n}\ln i$. Sketch a careful graph of $y = \ln x$, and by drawing in geometric figures above and below the graph, show that

$$\sum_{i=1}^{n}\ln i - \frac{1}{2}\ln n \le \int_1^n \ln x\,dx \le \sum_{i=1}^{n}\ln i.$$

Based on your drawing, which inequality do you think is tighter? Use integration by parts to evaluate the integral. What bounds on $n!$ can you get from these inequalities? Which one do you think is tighter? How does it compare to Stirling's approximation? What big Oh bound can you get on $n!$?

5.6 Conditional Expectations, Recurrences and Algorithms

Probability is a very important tool in algorithm design. We have already seen two important examples in which it is used—primality testing and hashing. In this section we will study several more examples of probabilistic analysis in algorithms. We will focus on computing the running time of various algorithms. When the running time of an algorithm is different for different inputs of the same size, we can think of the running time of the algorithm as a random variable on the sample space of inputs and analyze the expected running time of the algorithm. This gives us a different understanding from studying just the worst case running time for an input of a given size. We will then consider *randomized algorithms*, algorithms that depend on choosing something randomly, and see how we can use recurrences to give bounds on their expected running times as well.

For randomized algorithms, it will be useful to have access to a function which generates random numbers. We will assume that we have a function `randint(i,j)`, which generates a random integer uniformly between i and j (inclusive) [this means it is equally likely to be any number between i and j] and `rand01()`, which generates a random real number, uniformly between 0 and 1 [this means that given any two pairs of real numbers (r_1, r_2) and (s_1, s_2) with $r_2 - r_1 = s_2 - s_1$ and r_1, r_2, s_1 and s_2 all between 0 and 1, our random number is just as likely to be between r_1 and r_2 as it is to be between s_1 and s_2]. Functions such as `randint` and `rand01` are called *random number generators*. A great deal of number theory goes into the construction of good random number generators.

When Running Times Depend on more than Size of Inputs

Exercise 5.6-1 Let A be an array of length $n-1$ (whose elements are chosen from some ordered set), sorted into increasing order. Let b be another element of that ordered set that we want to insert into A to get a sorted array of length n. Assuming that the elements of A and b are chosen randomly, what is the expected number of elements of A that have to be shifted one place to the right to let us insert b?

Exercise 5.6-2 Let $A(1:n)$ denote the elements in positions 1 to n of the array A. A recursive description of insertion sort is that to sort $A(1:n)$, first we sort $A(1:n-1)$, and then we insert $A(n)$, by shifting the elements greater than $A(n)$ each one place to the right and then inserting the original value of $A(n)$ into the place we have opened up. If $n = 1$ we do nothing. Let $S_j(A(1:j))$ be the time needed to sort the portion of A from place 1 to place j, and let $I_j(A(1:j), b)$ be the time needed to insert the element b into a sorted list originally in the first j positions of A to give a sorted list in the first $j+1$ positions of A. Note that S_j and I_j depend on the actual array A, and not just on the value of j. Use S_j and I_j to describe the time needed to use insertion sort to sort $A(1:n)$ in terms of the time needed to sort $A(1:n-1)$. Don't forget that it is necessary to copy the element in position i of A into a variable b before moving elements of $A(1:i-1)$ to the right to make a place for it, because this moving process will write over $A(i)$. Let $T(n)$ be the expected value of S_n; that is, the expected running time of insertion sort on a list of n items. Write a recurrence for $T(n)$ in terms of $T(n-1)$ by taking expected values in the equation that corresponds to your previous description of the time needed to use insertion sort on a particular array. Solve your recurrence relation in big-Θ terms.

If X is the random variable with $X(A, b)$ equal to the number of items we need to move one place to the right in order to insert b into the resulting empty slot in A, then X takes on the values $0, 1, \ldots, n-1$ with equal probability $1/n$. Thus we have

$$E(x) = \sum_{i=0}^{n-1} i\frac{1}{n} = \frac{1}{n}\sum_{i=0}^{n-1} i = \frac{1}{n}\frac{(n-1)n}{2} = \frac{n-1}{2}.$$

Using $S_j(A(1:j))$ to stand for the time to sort the portion of the array A from places 1 to j by insertion sort, and $I_j(A(1:j), b)$ to stand for the time needed to insert b into a sorted list in the first j positions of the array A, moving all items larger than j to the right one place and putting b into the empty slot, we can write that for insertion sort

$$S_n(A(1:n)) = S_{n-1}(A(1:n-1)) + I_{n-1}(A(1:n-1), A(n)) + c_1.$$

We have included the constant term c_1 for the time it takes to copy the value of $A(n)$ into some variable b, because we will overwrite $A(n)$ in the process of moving items one place to the right. Using the additivity of expected values, we get

$$E(S_n) = E(S_{n-1}) + E(I_{n-1}) + E(c_1).$$

Using $T(n)$ for the expected time to sort $A(1:n)$ by insertion sort, and the result of the previous exercise, we get

$$T(n) = T(n-1) + c_2\frac{n-1}{2} + c_1.$$

where we include the constant c_2 because the time needed to do the insertion is going to be proportional to the number of items we have to move plus the time needed to copy the value of $A(n)$ into the appropriate slot (which we will assume we have included in c_1). We can say that $T(1) = 1$ (or some third constant) because with a list of size 1 we have to realize it has size 1, and then do nothing. It might be more realistic to write

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

and

$$T(n) \geq T(n-1) + c'n,$$

because the time needed to do the insertion may not be exactly proportional to the number of items we need to move, but might depend on implementation details. By iterating the recurrence or drawing a recursion tree, we see that $T(n) = \Theta(n^2)$. (We could also give an inductive proof.) Since the best-case time of insertion sort is $\Theta(n)$ and the worst case time is $\Theta(n^2)$, it is interesting to know that the expected case is much closer to the worst-case than the best case.

Conditional Expected Values

Our next example is cooked up to introduce an idea that we often use in analyzing the expected running times of algorithms, especially randomized algorithms.

Exercise 5.6-3 I have two nickels and two quarters in my left pocket and 4 dimes in my right pocket. Suppose I flip a penny and take two coins from my left pocket if it is heads, and two coins from my right pocket if it is tails. Assuming I am equally likely to choose any coin in my pocket at any time, what is the expected amount of money that I draw from my pocket?

You could do this problem by drawing a tree diagram or by observing that the outcomes can be modeled by three tuples in which the first entry is heads or tails, and the second and third entries are coins. Thus our sample space is HNQ, HQN, HQQ, HNN, TDD The probabilities of these outcomes are $\frac{1}{6}$, $\frac{1}{6}$, $\frac{1}{12}$, $\frac{1}{12}$, and $\frac{1}{2}$ respectively. Thus our expected value is

$$30\frac{1}{6} + 30\frac{1}{6} + 50\frac{1}{12} + 10\frac{1}{12} + 20\frac{1}{2} = 25.$$

Here is a method that seems even simpler. If the coin comes up heads, I have an expected value of 15 cents on each draw, so with probability 1/2, our expected value is 30 cents. If the coin comes up tails, I have an expected value of ten cents on each draw, so with probability 1/2 our expected value is 20 cents. Thus it is natural to expect that our expected value is $\frac{1}{2}30 + \frac{1}{2}20 = 25$ cents. In fact, if we group together the 4 outcomes with an H first, we see that their contribution to the expected value is 15 cents, which is 1/2 times 30, and if we look at the single element which has a T first, then its contribution to the sum is 10 cents, which is half of 20 cents.

In this second view of the problem, we took the probability of heads times the expected value of our draws, given that the penny came up heads, plus the probability of tails times the expected value of our draws, given that the penny came came up tails. In particular, we were using a new (and as yet undefined) idea of *conditional expected value.* To get the conditional expected value if our penny comes up heads, we could create a new sample space with four outcomes, NQ, QN, NN, QQ, with probabilities $\frac{1}{3}$, $\frac{1}{3}$, $\frac{1}{6}$, and $\frac{1}{6}$. In this sample space the expected amount of money we draw in two draws is 30 cents (15 cents for the first draw plus 15 cents for the second), so we would say the conditional expected value of our draws, given that the penny came up heads, was 30 cents. With a one-element sample space $\{DD\}$, we see that we would say that the conditional expected value of our draws, given that the penny came up tails, is 20 cents.

How do we define conditional expected value? Rather than create a new sample space as we did above, we use the idea of a new sample space (as we did in discovering a good definition for conditional probability) to lead us to a good definition for conditional expected value. In particular, to get the conditional expected value of X given that an event F has happened we use our conditional probability weights for the elements of F, namely $P(s)/P(F)$ is the weight for the element s of F, and pretend F is our sample space. Thus we define the **conditional expected value** of X given F by

$$E(X|F) = \sum_{x:s \in F} X(x)\frac{P(x)}{P(F)}. \tag{5.40}$$

Remember that we defined the expected value of a random variable X with values $x_1, x_2, \ldots x_k$ by

$$E(X) = \sum_{i=1}^{k} x_i P(X = x_i),$$

where $X = x_i$ stands for the event that X has the value x_i. Using our standard notation for conditional probabilities, $P(X = x_i|F)$ stands for the conditional probability of the event $X = x_i$ given the event F. This lets us rewrite Equation 5.40 as

$$E(X|F) = \sum_{i=1}^{k} x_i P(X = x_i|F).$$

Theorem 5.22 *Let X be a random variable defined on a sample space S and let F_1, F_2, $\ldots F_n$ be disjoint events whose union is S (i.e. a partition of S). Then*

$$E(X) = \sum_{i=1}^{n} E(X|F_i)P(F_i).$$

Proof: The proof is simply an exercise in applying definitions. ■

Randomized algorithms

Exercise 5.6-4 Consider an algorithm that, given a list of n numbers, prints them all out. Then it picks a random integer between 1 and 3. If the number is 1 or 2, it stops. If the number is 3 it starts again from the beginning. What is the expected running time of this algorithm?

Exercise 5.6-5 Consider the following variant on the previous algorithm:

```
funnyprint(n)
if (n == 1)
     return
for i = 1 to n
     print i
x = randint(1,n)
if (x > n/2)
     funnyprint(n/2)
else
     return
```

What is the expected running time of this algorithm?

For Exercise 5.6-4, with probability 2/3 we will print out the numbers and quit, and with probability 1/3 we will run the algorithm again. Using Theorem 5.22, we see that if $T(n)$ is the expected running time on a list of length n, then there is a constant c such that

$$T(n) = \frac{2}{3}cn + \frac{1}{3}(cn + T(n)),$$

which gives us $\frac{2}{3}T(n) = cn$. This simplifies to $T(n) = \frac{3}{2}cn$.

Another view is that we have an independent trials process, with success probability 2/3 where we stop at the first success, and for each round of the independent trials process we spend $\Theta(n)$ time. Letting T be the running time (note that T is a random variable on the sample space $1, 2, 3$ with probabilities $\frac{1}{3}$ for each member) and R be the number of rounds, we have that

$$T = R \cdot \Theta(n)$$

and so

$$E(T) = E(R)\Theta(n).$$

Note that we are applying Theorem 5.10 since in this context $\Theta(n)$ behaves as if it were a constant[7], since n does not depend on R. By Lemma 5.12, we have that $E(R) = 3/2$ and so $E(T) = \Theta(n)$.

In Exercise 5.6-5, we have a recursive algorithm, and so it is appropriate to write down a recurrence. We can let $T(n)$ stand for the *expected* running time of the algorithm on an input of size n. Notice how we are changing back and forth between letting T stand for the running time of an algorithm and the expected running time of an algorithm. Usually we use T to stand for the quantity of most interest to us, either running time if that makes sense, or expected running time (or maybe worst-case running time) if the actual running time might vary over different inputs of size n. The nice thing will be that once we write down a recurrence for the expected running time of an algorithm, the methods for solving it will be those for we have already learned for solving recurrences. For the problem at hand, we immediately get that with probability 1/2 we will be spending n units of time (we should really say $\Theta(n)$ time), and then terminating, and with probability 1/2 we will spend n units of time and then recurse on a problem of size $n/2$. Thus using Theorem 5.22, we get that

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

Including a base case of $T(1) = 1$, we get that

$$T(n) = \begin{cases} \frac{1}{2}T(n/2) + n & \text{if } n > 1 \\ 1 & \text{if } n = 1 \end{cases}.$$

A simple proof by induction shows that $T(n) = \Theta(n)$. Note that the Master Theorem (as we originally stated it) doesn't apply here, since $a < 1$. However, one could also observe that the solution to this recurrence is no more than the solution to the recurrence $T(n) = T(n/2) + n$, and then apply the Master Theorem.

Selection revisited

We now return to the selection algorithm from Section 4.6. The purpose of the algorithm is to select the ith smallest element in a set with some underlying order. Recall that in this algorithm, we first picked an an element p in the middle half of the set, that is, one whose value was simultaneously larger than at least 1/4 of the items and smaller than at least 1/4 of the items. We used p to partition the items into two sets and then recursed on one of the two sets. If you recall, we worked very hard to find an item in the middle half, so that our partitioning would

[7]What we mean here is that $T \geq Rc_1n$ for some constant c_1 and $T \leq Rc_2n$ for some other constant c_2. Then we apply Theorem 5.10 to both these inequalities, using the fact that if $X > Y$, then $E(X) > E(Y)$ as well.

work well. It is natural to try instead to just pick a partition element at random, because, with probability 1/2, this element will be in the middle half. We can extend this idea to the following algorithm:

```
RandomSelect(A,i,n)
(selects the ith smallest element in set A, where n = |A| )
if (n = 1)
     return the one item in A
else
     p = randomElement(A)
     Let H be the set of elements greater than p
     Let L be the set of elements less than or equal to p
     If (H is empty)
          put p in H
     if (i ≤ |L|)
          Return RandomSelect(L, i, |L|)
     else
          Return RandomSelect(H, i − |L|, |H|).
```

Here randomElement(A) returns one element from A uniformly at random. We use this element as our partition element; that is, we use it to divide A into sets L and H with every element less than the partition element in L and every element greater than it in H. We add the special case when H is empty, to ensure that both recursive problems have size strictly less than n. This simplifies a detailed analysis, but is not strictly necessary. At the end of this section we will show how to get a recurrence that describes fairly precisely the time needed to carry out this algorithm. However, by being a bit less precise, we can still get the same big-O upper bound with less work.

When we choose our partition element, half the time it will be between $\frac{1}{4}n$ and $\frac{3}{4}n$. Then when we partition our set into H and L, each of these sets will have no more than $\frac{3}{4}n$ elements. The other half of the time each of H and L will have no more than n elements. In any case, the time to partition our set into H and L is $O(n)$. Thus we may write

$$T(n) \le \begin{cases} \frac{1}{2}T(\frac{3}{4}n) + \frac{1}{2}T(n) + bn & \text{if } n > 1 \\ d & \text{if } n = 1. \end{cases}$$

We may rewrite the recursive part of the recurrence as

$$\frac{1}{2}T(n) \le \frac{1}{2}T\left(\frac{3}{4}n\right) + bn,$$

or

$$T(n) \le T\left(\frac{3}{4}n\right) + 2bn = T\left(\frac{3}{4}n\right) + b'n.$$

Notice that it is possible (but unlikely) that each time our algorithm chooses a pivot element, it chooses the worst one possible, in which case the selection process could take n rounds, and thus take time $\Theta(n^2)$. Why, then, is it of interest? It involves far less computation than finding the median of medians, and its expected running time is still $\Theta(n)$. Thus it is reasonable to suspect that on the average, it would be significantly faster than the deterministic process. In fact, with good implementations of both algorithms, this will be the case.

Exercise 5.6-6 Why does every solution to the recurrence

$$T(n) \le T\left(\frac{3}{4}n\right) + b'n$$

have $T(n) = O(n)$?

By the master theorem we know that any solution to this recurrence is $O(n)$, giving a proof of our next Theorem.

Theorem 5.23 *Algorithm RandomSelect has expected running time $O(n)$.*

Quicksort

There are many algorithms that will efficiently sort a list of n numbers. The two most common sorting algorithms that are guaranteed to run in $O(n \log n)$ time are MergeSort and HeapSort. However, there is another algorithm, Quicksort, which, while having a worst-case running time of $O(n^2)$, has an expected running time of $O(n \log n)$. Moreover, when implemented well, it tends to have a faster running time than MergeSort or HeapSort. Since many computer operating systems and programs come with Quicksort built in, it has become the sorting algorithm of choice in many applications. In this section, we will see why it has expected running time $O(n \log n)$. We will not concern ourselves with the low-level implementation issues that make this algorithm the fastest one, but just with a high-level description.

Quicksort actually works similarly to the RecursiveSelect algorithm of the previous subsection. We pick a random element, and then use it to partition the set of items into two sets L and H. In this case, we don't recurse on one or the other, but recurse on both, sorting each one. After both L and H have been sorted, we just concatenate them to get a sorted list. (In fact, Quicksort is usually done "in place" by pointer manipulation and so the concatenation just happens.) Here is a pseudocode description of Quicksort:

```
Quicksort(A,n)
if (n = 1)
    return the one item in A
else
    p = randomElement(A)
    Let H be the set of elements greater than p; Let h = |H|
    Let L be the set of elements less than or equal to p; Let ℓ = |L|
    If (H is empty)
        put p in H
    A1 = QuickSort(H,h)
    A2 = QuickSort(L,ℓ)
    return the concatenation of A1 and A2.
```

There is an analysis of Quicksort similar to the detailed analysis of RecursiveSelect at the end of the section, and this analysis is a problem at the end of the section. Instead, based on the preceding analysis of RandomSelect we will think about modifying the algorithm a bit in order to make the analysis easier. First, consider what would happen if the random element was the median each time. Then we would be solving two subproblems of size $n/2$, and would have the recurrence

$$T(n) = \begin{cases} 2T(n/2) + O(n) & \text{if } n > 1 \\ O(1) & \text{if } n = 1 \end{cases}$$

and we know by the master theorem that all solutions to this recurrence have $T(n) = O(n \log n)$. In fact, we don't need such an even division to guarantee such performance.

Exercise 5.6-7 Suppose you had a recurrence of the form

$$T(n) \leq \begin{cases} T(a_n n) + T((1-a_n)n) + cn & \text{if } n > 1 \\ d & \text{if } n = 1, \end{cases}$$

where a_n is between $1/4$ and $3/4$. Show that all solutions of a recurrence of this form have $T(n) = O(n \log n)$. What do we really need to assume about a_n in order to prove this upper bound?

We can prove that $T(n) = O(n \log n)$ by induction, or via a recursion tree, noting that there are $O(\log n)$ levels, and each level has at most $O(n)$ work. (The details of the recursion tree are complicated somewhat by the fact that a_n varies with n, while the details of an inductive proof simply use the fact that a_n and $1 - a_n$ are both no more than $3/4$.) So long as we know there is some positive number $a < 1$ such that $a_n < a$ for every n, then we know we have at most $\log_{(1/a)} n$ levels in a recursion tree, with at most cn units of work per level for some constant c, and thus we have the same upper bound in big-O terms.

What does this tell us? As long as our problem splits into two pieces, each having size at least $1/4$ of the items, Quicksort will run in $O(n \log n)$ time. Given this, we will modify our algorithm to enforce this condition. That is, if we choose a pivot element p that is not in the middle half, we will just pick another one. This leads to the following algorithm:

```
Slower Quicksort(A,n)
if (n = 1)
    return the one item in A
else
    Repeat
        p = randomElement(A)
        Let H be the set of elements greater than p; Let h = |H|
        Let L be the set of elements less than or equal to p; Let ℓ = |L|
    Until (|H| ≥ n/4) and (|L| ≥ n/4)
    A_1 = QuickSort(H,h)
    A_2 = QuickSort(L,ℓ)
    return the concatenation of A_1 and A_2
```

Now let's analyze this algorithm. Let r be the number of times we execute the loop to pick p, and let $a_n n$ be the position of the pivot element. Then if $T(n)$ is the expected running time for a list of length n, then for some constant b

$$T(n) \leq E(r)bn + T(a_n n) + T((1-a_n)n),$$

since each iteration of the loop takes $O(n)$ time. Note that we take the expectation of r, because $T(n)$ stands for the expected running time on a problem of size n. Fortunately, $E(r)$ is simple to compute, it is just the expected time until the first success in an independent trials process with success probability 1/2. This is 2. So we get that the running time of Slower Quicksort satisfies the recurrence

$$T(n) \le \begin{cases} T(a_n n) + T((1-a_n))n + b'n & \text{if } n > 1 \\ d & \text{if } n = 1 \end{cases},$$

where a_n is between 1/4 and 3/4. Thus by Exercise 5.6-7 the running time of this algorithm is $O(n \log n)$.

As another variant on the same theme, observe that looping until we have$(|H| \ge n/4$ and $|L| \ge n/4$, is effectively the same as choosing p, finding H and L and then calling Slower Quicksort(A,n) once again if either H or L has size less than $n/4$. Then since with probability 1/2 the element p is between $n/4$ and $3n/4$, we can write

$$T(n) \le \frac{1}{2}T(n) + \frac{1}{2}(T(a_n n) + T((1-a_n)n) + bn),$$

which simplifies to

$$T(n) \le T(a_n n) + T((1-a_n)n) + 2bn,$$

or

$$T(n) \le T(a_n n) + T((1-a_n)n) + b'n.$$

Again by Exercise 5.6-7 the running time of this algorithm is $O(n \log n)$.

Further, it is straightforward to see that the expected running time of Slower Quicksort is no less than half that of Quicksort (and, incidentally, no more than twice that of Quicksort) and so we have shown:

Theorem 5.24 *Quicksort has expected running time $O(n \log n)$.*

A more exact analysis of RandomSelect

Recall that our analysis of the RandomSelect was based on using $T(n)$ as an upper bound for $T(|H|)$ or $T(|L|)$ if either the set H or the set L had more than $3n/4$ elements. Here we show how one can avoid this assumption. The kinds of computations we do here are the kind we would need to do if we wanted to try to actually get bounds on the constants implicit in our big-O bounds.

Exercise 5.6-8 Explain why, if we pick the kth element as the random element in RandomSelect ($k \ne n$), our recursive problem is of size no more than $\max\{k, n-k\}$.

If we pick the kth element, then we recurse either on the set L, which has size k, or on the set H, which has size $n-k$. Both of these sizes are at most $\max\{k, n-k\}$. (If we pick the nth element, then $k = n$ and thus L actually has size $k-1$ and H has size $n-k+1$.)

Now let X be the random variable equal to the rank of the chosen random element (e.g. if the random element is the third smallest, $X = 3$.) Using Theorem 5.22 and the solution to Exercise 5.6-8, we can write that

$$T(n) \le \begin{cases} \sum_{k=1}^{n-1} P(X=k)(T(\max\{k, n-k\}) + bn) + P(X=n)(T(\max\{1, n-1\} + bn) & \text{if } n > 1 \\ d & \text{if } n = 1. \end{cases}$$

Since X is chosen uniformly between 1 and n, $P(X = k) = 1/n$ for all k. Ignoring the base case for a minute, we get that

$$\begin{aligned} T(n) &\le \sum_{k=1}^{n-1} \frac{1}{n}(T(\max\{k, n-k\}) + bn) + \frac{1}{n}(T(n-1) + bn) \\ &= \frac{1}{n}\left(\sum_{k=1}^{n-1} T(\max\{k, n-k\})\right) + bn + \frac{1}{n}(T(n-1) + bn). \end{aligned}$$

Now if n is odd and we write out $\sum_{k=1}^{n-1} T(\max\{k, n-k\})$, we get

$$T(n-1) + T(n-2) + \cdots + T(\lceil n/2 \rceil) + T(\lceil n/2 \rceil) + \cdots + T(n-2) + T(n-1),$$

which is just $2\sum_{k=\lceil n/2 \rceil}^{n-1} T(k)$. If n is even and we write out $\sum_{k=1}^{n-1} T(\max\{k, n-k\})$, we get

$$T(n-1) + T(n-2) + \cdots + T(n/2) + T(1 + n/2) + \cdots + T(n-2) + T(n-1),$$

which is less than $2\sum_{k=n/2}^{n-1} T(k)$. Thus we can replace our recurrence by

$$T(n) \le \begin{cases} \frac{2}{n}\left(\sum_{k=n/2}^{n-1} T(k)\right) + \frac{1}{n}T(n-1) + bn & \text{if } n > 1 \\ d & \text{if } n = 1. \end{cases} \tag{5.41}$$

If n is odd, the lower limit of the sum is a half-integer, so the possible integer values of the dummy variable k run from $\lceil n/2 \rceil$ to $n - 1$. Since this is the natural way to interpret a fractional lower limit, and since it corresponds to what we wrote in both the n even and n odd case above, we adopt this convention.

Exercise 5.6-9 Show that every solution to the recurrence in Equation 5.41 has $T(n) = O(n)$.

We can prove this by induction. We try to prove that $T(n) \le cn$ for some constant c. By the natural inductive hypothesis, we get that

$$\begin{aligned} T(n) &\le \frac{2}{n}\left(\sum_{k=n/2}^{n-1} ck\right) + \frac{1}{n}c(n-1) + bn \\ &= \frac{2}{n}\left(\sum_{k=1}^{n-1} ck - \sum_{k=1}^{n/2-1} ck\right) + \frac{1}{n}c(n-1) + bn \\ &\le \frac{2c}{n}\left(\frac{(n-1)n}{2} - \frac{(\frac{n}{2}-1)\frac{n}{2}}{2}\right) + c + bn \\ &= \frac{2c}{n}\frac{\frac{3n^2}{4} - \frac{n}{2}}{2} + c + bn \\ &= \frac{3}{4}cn + \frac{c}{2} + bn \\ &= cn - (\frac{1}{4}cn - bn - \frac{c}{2}) \end{aligned}$$

Notice that so far, we have only assumed that there is some constant c such that $T(k) < ck$ for $k < n$. We can choose a larger c than the one given to us by this assumption without changing the inequality $T(k) < ck$. By choosing c so that $\frac{1}{4}cn - bn - \frac{c}{2}$ is nonnegative (for example $c \geq 8b$ makes this term at least $bn - 2b$ which is nonnegative for $n \geq 2$), we conclude the proof, and have another proof of Theorem 5.23.

This kind of careful analysis arises when we are trying to get an estimate of the constant in a big-O bound (which we decided not to do in this case).

Important Concepts, Formulas, and Theorems

1. *Expected Running Time.* When the running time of an algorithm is different for different inputs of the same size, we can think of the running time of the algorithm as a random variable on the sample space of inputs and analyze the expected running time of the algorithm. This gives us a different understanding from studying just the worst case running time.

2. *Randomized Algorithm.* A*randomized algorithm* is an algorithm that depends on choosing something randomly.

3. *Random Number Generator.* A random number generator is a procedure that generates a number that appears to be chosen at random. Usually the designer of a random number generator tries to generate numbers that appear to be uniformly distributed.

4. *Insertion Sort.* A recursive description of insertion sort is that to sort $A(1:n)$, first we sort $A(1:n-1)$, and then we insert $A(n)$, by shifting the elements greater than $A(n)$ each one place to the right and then inserting the original value of $A(n)$ into the place we have opened up. If $n = 1$ we do nothing.

5. *Expected Running Time of Insertion Sort.* If $T(n)$ is the expected time to use insertion sort on a list of length n, then there are constants c and c' such that $T(n) \leq T(n-1) + cn$ and $T(n) \geq T(n-1) + c'n$. This means that $T(n) = \Theta(n^2)$. However the best case running time of insertion sort is $\Theta(n)$.

6. *Conditional Expected Value.* We define the *conditional expected value* of X given F by $E(X|F) = \sum_{x:x\in F} X(x)\frac{P(x)}{P(F)}$. This is equivalent to $E(X|F) = \sum_{i=1}^{k} x_i P(X = x_i|F)$.

7. *Randomized Selection Algorithm.* In the randomized selection algorithm to select the ith smallest element of a set A, we randomly choose a pivot element p in A, divide the rest of A into those elements that come before p (in the underlying order of A) and those that come after, put the pivot into the smaller set, and then recursively apply the randomized selection algorithm to find the appropriate element of the appropriate set.

8. *Running Time of Randomized Select.* Algorithm RandomSelect has expected running time $O(n)$. Because it does less computation than the deterministic selection algorithm, on the average a good implementation will run faster than a good implementation of the deterministic algorithm, but the worst case behavior is $\Theta(n^2)$.

9. *Quicksort.* Quicksort is a sorting algorithm in which we randomly choose a pivot element p in A, divide the rest of A into those elements that come before p (in the underlying order of A) and those that come after, put the pivot into the smaller set, and then recursively apply the Quicksort algorithm to sort each of the smaller sets, and concatenate the two sorted lists. We do nothing if a set has size one.

10. *Running Time of Quicksort.* Quicksort has expected running time $O(n \log n)$. It has worst case running time $\Theta(n^2)$. Good implementations of Quicksort have proved to be faster on the average than good implementations of other sorting algorithms.

Problems

1. Given an array A of length n (chosen from some set that has an underlying ordering), we can select the largest element of the array by starting out setting $L = A(1)$, and then comparing L to the remaining elements of the array one at a time, replacing L by $A(i)$ if $A(i)$ is larger than L. Assume that the elements of A are randomly chosen. For $i > 1$, let X_i be 1 if element i of A is larger than any element of $A(1 : i-1)$. Let $X_1 = 1$. Then what does $X_1 + X_2 + \cdots + X_n$ have to do with the number of times we assign a value to L? What is the expected number of times we assign a value to L?

2. Let $A(i : j)$ denote the array of items in positions i through j of the Array A. In selection sort, we use the method of Exercise 5.6-1 to find the largest element of the array A and its position k in the array, then we exchange the elements in position k and n of Array A, and we apply the same procedure recursively to the array $A(1 : n-1)$. (Actually we do this if $n > 1$; if $n = 1$ we do nothing.) What is the expected total number of times we assign a value to L in the algorithm selection sort?

3. Show that if H_n stands for the nth harmonic number, then

$$H_n + H_{n-1} + \cdots + H_2 = \Theta(n \log n).$$

4. In a card game, we remove the Jacks, Queens, Kings, and Aces from a deck of ordinary cards and shuffle them. You draw a card. If it is an Ace, you are paid a dollar and the game is repeated. If it is a Jack, you are paid two dollars and the game ends; if it is a Queen, you are paid three dollars and the game ends; and if it is a King, you are paid four dollars and the game ends. What is the maximum amount of money a rational person would pay to play this game?

5. Why does every solution to $T(n) \le T(\frac{2}{3}n) + bn$ have $T(n) = O(n)$?

6. Show that if in Algorithm Random Select we remove the instruction

```
If H is empty
     put p in H,
```

then if $T(n)$ is the expected running time of the algorithm, there is a constant b such that $T(n)$ satisfies the recurrence

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

Show that if $T(n)$ satisfies this recurrence, then $T(n) = O(n)$.

7. Suppose you have a recurrence of the form

$$T(n) \le T(a_n n) + T((1 - a_n)n) + bn \text{ if } n > 1,$$

where a_n is between $\frac{1}{5}$ and $\frac{4}{5}$. Show that all solutions to this recurrence are of the form $T(n) = O(n \log n)$.

8. Prove Theorem 5.22.

9. A tighter (up to constant factors) analysis of Quicksort is possible by using ideas very similar to those that we used for the randomized selection algorithm. More precisely, we use Theorem 5.6.1, similarly to the way we used it for select. Write down the recurrence you get when you do this. Show that this recurrence has solution $O(n \log n)$. In order to do this, you will probably want to prove that $T(n) \le c_1 n \log n - c_2 n$ for some constants c_1 and c_2.

10. It is also possible to write a version of the randomized Selection algorithm analogous to Slower Quicksort. That is, when we pick out the random pivot element, we check if it is in the middle half and discard it if it is not. Write this modified selection algorithm, give a recurrence for its running time, and show that this recurrence has solution $O(n)$.

11. One idea that is often used in selection is that instead of choosing a random pivot element, we choose three random pivot elements and then use the median of these three as our pivot. What is the probability that a randomly chosen pivot element is in the middle half? What is the probability that the median of three randomly chosen pivot elements is in the middle half? Does this justify the choice of using the median of three as pivot?

12. Is the expected running time of Quicksort $\Omega(n \log n)$?

13. A random binary search tree on n keys is formed by first randomly ordering the keys, and then inserting them in that order. Explain why in at least half the random binary search trees, both subtrees of the root have between $\frac{1}{4}n$ and $\frac{3}{4}n$ keys. If $T(n)$ is the expected height of a random binary search tree on n keys, explain why $T(n) \le \frac{1}{2}T(n) + \frac{1}{2}T(\frac{3}{4}n) + 1$. (Think about the **definition** of a binary tree. It has a root, and the root has two subtrees! What did we say about the possible sizes of those subtrees?) What is the expected height of a one node binary search tree? Show that the expected height of a random binary search tree is $O(\log n)$.

14. The expected time for an unsuccessful search in a random binary search tree on n keys (see Problem 13 for a definition) is the expected depth of a leaf node. Arguing as in Problem 13 and the second proof of Theorem 5.6.2, find a recurrence that gives an upper bound on the expected depth of a leaf node in a binary search tree and use it to find a big Oh upper bound on the expected depth of a leaf node.

15. The expected time for a successful search in a random binary search tree on n nodes (see problem 13 for a definition) is the expected depth of a node of the tree. With probability $\frac{1}{n}$ the node is the root, which has depth 0; otherwise the expected depth is one plus the expected depth of one of its subtrees. Argue as in Problem 13 and the first proof of Theorem 5.23 to show that if $T(n)$ is the expected depth of a node in a binary search tree, then $T(n) \le \frac{n-1}{n}(\frac{1}{2}T(n) + \frac{1}{2}T(\frac{3}{4}n)) + 1$. What big Oh upper bound does this give you on the expected depth of a node in a random binary search tree on n nodes?

16. Consider the following code for searching an array A for the maximum item:

    $max = -\infty$
    for $i = 1$ to n
        if $(A[i] > max)$
            $max = A[i]$

    If A initially consists of n nodes in a random order, what is the expected number of times that the line $max = A[i]$ is executed? (Hint: Let X_i be the number of times that $max = A[i]$ is executed in the ith iteration of the loop.)

17. You are a contestant in the game show "Let's make a Deal." In this game show, there are three curtains. Behind one of the curtains is a new car, and behind the other two are cans of spam. You get to pick one of the curtains. After you pick that curtain, the emcee, Monte Hall, who we assume knows where the car is, reveals what is behind one of the curtains that you did not pick, showing you some cans of spam. He then asks you if you would like to switch your choice of curtain. Should you switch? Why or why not? Please answer this question carefully. You have all the tools needed to answer it, but several math Ph.D.'s are on record (in Parade Magazine) giving the wrong answer.

5.7 Probability Distributions and Variance

Distributions of random variables

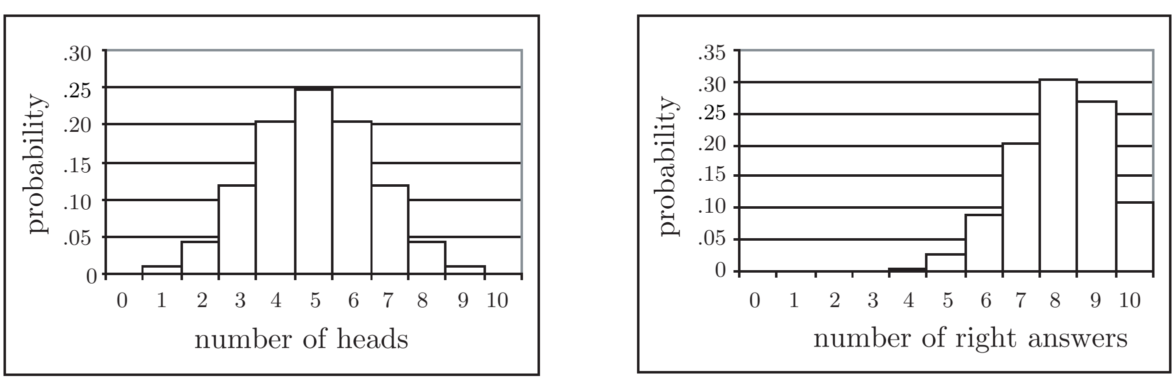
We have given meaning to the phrase expected value. For example, if we flip a coin 100 times, the expected number of heads is 50. But to what extent do we expect to see 50 heads. Would it be surprising to see 55, 60 or 65 heads instead? To answer this kind of question, we have to analyze how much we expect a random variable to deviate from its expected value. We will first see how to analyze graphically how the values of a random variable are distributed around its expected value. The *distribution function* D of a random variable X is the function on the values of X defined by

$$D(x) = P(X = x).$$

You probably recognize the distribution function from the role it played in the definition of expected value. The distribution function of the random variable X assigns to each value x of X the probability that X achieves that value. (Thus D is a function whose domain is the set off values of X.) When the values of X are integers, it is convenient to visualize the distribution function with a diagram called a *histogram*. In Figure 5.8 we show histograms for the distribution of the "number of heads" random variable for ten flips of a coin and the "number of right answers" random variable for someone taking a ten question test with probability .8 of getting a correct answer. What is a histogram? Those we have drawn are graphs which show for for each integer value x of X a rectangle of width 1, centered at x, whose height (and thus area) is proportional to the probability $P(X = x)$. Histograms can be drawn with non-unit width rectangles. When people draw a rectangle with a base ranging from $x = a$ to $x = b$, the area of the rectangle is the probability that X is between a and b.

The function $D(a, b) = P(a \leq X \leq b)$ is often called a *cumulative distribution function*. When sample spaces can be infinite, it doesn't always make sense to assign probability weights to individual members of our sample space, but cumulative distribution functions still make sense. Thus for infinite sample spaces, the treatment of probability is often based on random variables and their cumulative distribution functions. Histograms are a natural way to display information about the cumulative distribution function.

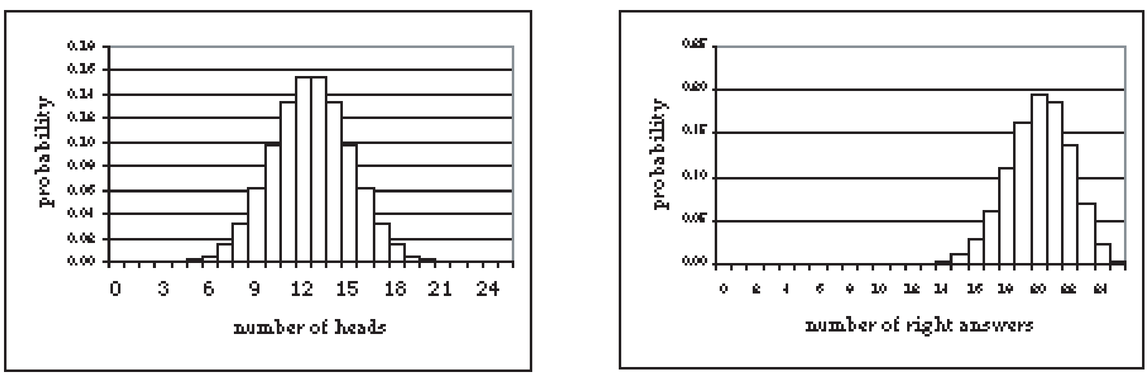
Figure 5.8: Two histograms.



From the histograms in Figure 5.8 you can see the difference between the two distributions.

You can also see that we can expect the number of heads to be somewhat near the expected number, though as few heads as 2 or as many as 8 are not out of the question. We see that the number of right answers tends to be clustered between 6 and ten, so in this case we can expect to be reasonably close to the expected value. With more coin flips or more questions, however, will the results spread out? Relatively speaking, should we expect to be closer to or farther from the expected value? In Figure 5.9 we show the results of 25 coin flips or 25 questions. The expected number of heads is 12.5. The histogram makes it clear that we can expect the vast majority of our results to have between 9 and 16 heads. Essentially all the results lie between 5 and 20 Thus the results are not spread as broadly (relatively speaking) as they were with just ten flips. Once again the test score histogram seems even more tightly packed around its expected value. Essentially all the scores lie between 14 and 25. While we can still tell the difference between the shapes of the histograms, they have become somewhat similar in appearance.

Figure 5.9: Histograms of 25 trials



In Figure 5.10 we have shown the thirty most relevant values for 100 flips of a coin and a 100 question test. Now the two histograms have almost the same shape, though the test histogram is still more tightly packed around its expected value. The number of heads has virtually no chance of deviating by more than 15 from its expected value, and the test score has almost no chance of deviating by more than 11 from the expected value. Thus the spread has only doubled, even though the number of trials has quadrupled. In both cases the curve formed by the tops of the rectangles seems quite similar to the bell shaped curve called the normal curve that arises in so many areas of science. In the test-taking curve, though, you can see a bit of difference between the lower left-hand side and the lower right hand side.

Since we needed about 30 values to see the most relevant probabilities for these curves, while we needed 15 values to see most of the relevant probabilities for independent trials with 25 items, we might predict that we would need only about 60 values to see essentially all the results in four hundred trials. As Figure 5.11 shows, this is indeed the case. The test taking distribution is still more tightly packed than the coin flipping distribution, but we have to examine it closely to find any asymmetry. These experiments are convincing, and they suggest that the spread of a distribution (for independent trials) grows as the square root of the number of trials, because each time we quadruple the number of elements, we double the spread. They also suggest there is some common kind of bell-shaped limiting distribution function for at least the distribution of successes in independent trials with two outcomes. However without a theoretical foundation we

Figure 5.10: One hundred independent trials

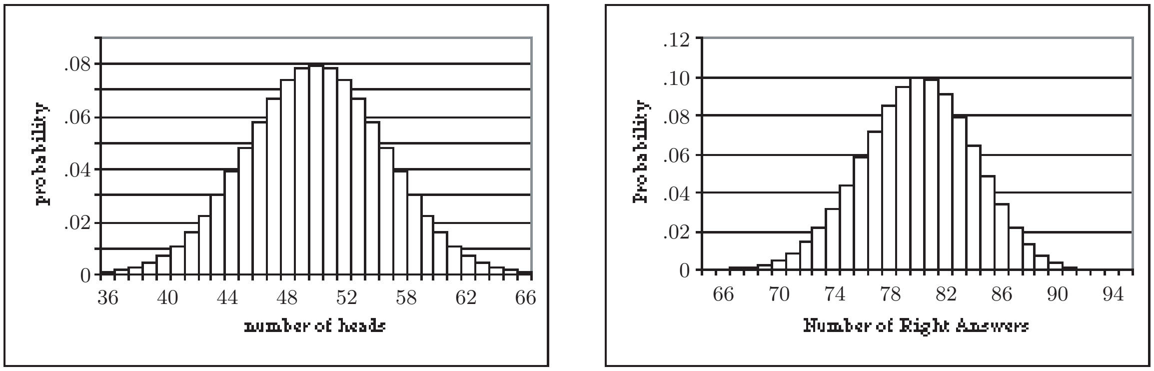
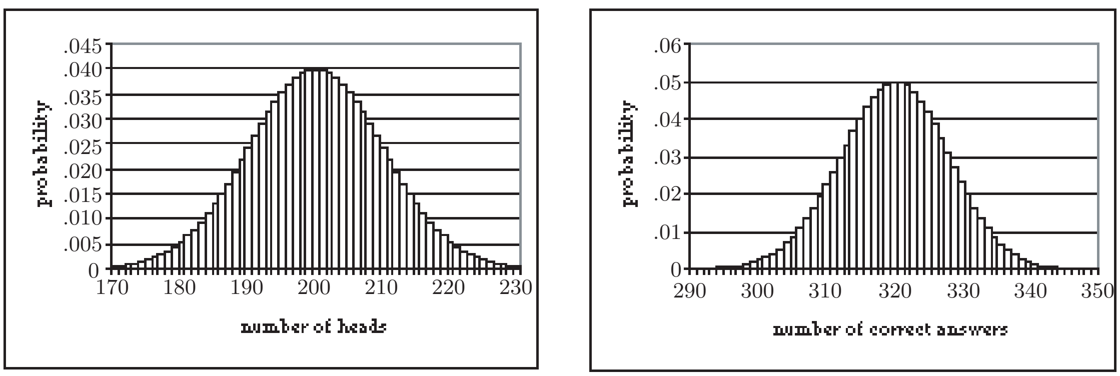


Figure 5.11: Four hundred independent trials



don't know how far the truth of our observations extends. Thus we seek an algebraic expression of our observations. This algebraic measure should somehow measure the difference between a random variable and its expected value.

Variance

Exercise 5.7-1 Suppose the X is the number of heads in four flips of a coin. Let Y be the random variable $X - 2$, the difference between X and its expected value. Compute $E(Y)$. Does it effectively measure how much we expect to see X deviate from its expected value? Compute $E(Y^2)$. Try repeating the process with X being the number of heads in ten flips of a coin and Y being $X - 5$.

Before answering these questions, we state a trivial, but useful, lemma (which appeared as Problem 9 in Section 5.4 of this chapter) and corollary showing that the expected value of an expectation is that expectation.

Lemma 5.25 *If X is a random variable that always takes on the value c, then $E(X) = c$.*

Proof: $E(X) = P(X = c) \cdot c = 1 \cdot c = c.$ ■

We can think of a constant c as a random variable that always takes on the value c. When we do, we will just write $E(c)$ for the expected value of this random variable, in which case our lemma says that $E(c) = c$. This lemma has an important corollary.

Corollary 5.26 $E(E(X)) = E(X)$.

Proof: When we think of $E(X)$ as a random variable, it has a constant value, μ. By Lemma 5.25 $E(E(x)) = E(\mu) = \mu = E(x)$. ■

Returning to Exercise 5.7-1, we can use linearity of expectation and Corollary 5.26 to show that

$$E(X - E(X)) = E(X) - E(E(X)) = E(X) - E(X) = 0. \tag{5.42}$$

Thus this is not a particularly useful measure of how close a random variable is to its expectation. If a random variable is sometimes above its expectation and sometimes below, you would like these two differences to somehow add together, rather than cancel each other out. This suggests we try to convert the values of $X - E(X)$ to positive numbers in some way and then take the expectation of these positive numbers as our measure of spread. There are two natural ways to make numbers positive, taking their absolute value and squaring them. It turns our that to prove things about the spread of expected values, squaring is more useful. Could we have guessed that? Perhaps, since we see that the spread seems to grow with the square root, and the square root isn't related to the absolute value in the way it is related to the squaring function. On the other hand, as you saw in the example, computing expected values of these squares from what we know now is time consuming. A bit of theory will make it easier.

We define the **variance** $V(X)$ of a random variable X as the expected value of $E\left((X - E(X))^2\right)$. We can also express this as a sum over the individual elements of the sample space S and get that

$$V(X) = E(X - E(X))^2 = \sum_{s:s\in S} P(s)(X(s) - E(X))^2. \tag{5.43}$$

Now let's apply this definition and compute the variance in the number X of heads in four flips of a coin. We have

$$V(X) = (0-2)^2 \cdot \frac{1}{16} + (1-2)^2 \cdot \frac{1}{4} + (2-2)^2 \cdot \frac{3}{8} + (3-2)^2 \cdot \frac{1}{4} + (4-2)^2 \cdot \frac{1}{16} = 1.$$

Computing the variance for ten flips of a coin involves some very inconvenient arithmetic. It would be nice to have a computational technique that would save us from having to figure out large sums if we want to compute the variance for ten or even 100 or 400 flips of a coin to check our intuition about how the spread of a distribution grows. We saw before that the expected value of a sum of random variables is the sum of the expected values of the random variables. This was very useful in making computations.

Exercise 5.7-2 What is the variance for the number of heads in one flip of a coin? What is the sum of the variances for four independent trials of one flip of a coin?

Exercise 5.7-3 We have a nickel and quarter in a cup. We withdraw one coin. What is the expected amount of money we withdraw? What is the variance? We withdraw two coins, one after the other without replacement. What is the expected amount of money we withdraw? What is the variance? What is the expected amount of money and variance for the first draw? For the second draw?

Exercise 5.7-4 Compute the variance for the number of right answers when we answer one question with probability .8 of getting the right answer (note that the number of right answers is either 0 or 1, but the expected value need not be). Compute the variance for the number of right answers when we answer 5 questions with probability .8 of getting the right answer. Do you see a relationship?

In Exercise 5.7-2 we can compute the variance

$$V(X) = (0 - \frac{1}{2})^2 \cdot \frac{1}{2} + (1 - \frac{1}{2})^2 \cdot \frac{1}{2} = \frac{1}{4}.$$

Thus we see that the variance for one flip is 1/4 and sum of the variances for four flips is 1. In Exercise 5.7-4 we see that for one question the variance is

$$V(X) = .2(0 - .8)^2 \, + \, .8(1 - .8)^2 = .16$$

For five questions the variance is

$$4^2 \cdot (.2)^5 \, + \, 3^2 \cdot 5 \cdot (.2)^4 \cdot (.8) \, + \, 2^2 \cdot 10 \cdot (.2)^3 \cdot (.8)^2 \, + \, 1^2 \cdot 10 \cdot (.2)^2 \cdot (.8)^3 \, + \\ 0^2 \cdot 5 \cdot (.2)^1 \cdot (.8)^4 \, + \, 1^2 \cdot (.8)^5 = .8.$$

The result is five times the variance for one question.

For Exercise 5.7-3 the expected amount of money for one draw is \$.15. The variance is

$$(.05 - .15)^2 \cdot .5 \, + \, (.25 - .15)^2 \cdot .5 = .01.$$

For removing both coins, one after the other, the expected amount of money is \$.30 and the variance is 0. Finally the expected value and variance on the first draw are \$.15 and .01 and the expected value and variance on the second draw are \$.15 and .01.

It would be nice if we had a simple method for computing variance by using a rule like "the expected value of a sum is the sum of the expected values." However Exercise 5.7-3 shows that the variance of a sum is not always the sum of the variances. On the other hand, Exercise 5.7-2 and Exercise 5.7-4 suggest such a result might be true for a sum of variances in independent trials processes. In fact slightly more is true. We say random variables X and Y are *independent* when the event that X has value x is independent of the event that Y has value y, regardless of the choice of x and y. For example, in n flips of a coin, the number of heads on flip i (which is 0 or 1) is independent of the number of heads on flip j. To show that the variance of a sum of independent random variables is the sum of their variances, we first need to show that the expected value of the product of two *independent* random variables is the product of their expected values.

Lemma 5.27 *If X and Y are independent random variables on a sample space S with values $x_1, x_2, \ldots, x_k$ and $y_1, y_2, \ldots, y_m$ respectively, then*

$$E(XY) = E(X)E(Y).$$

Proof: We prove the lemma by the following series of equalities. In going from (5.44) to (5.45), we use the fact that X and Y are independent; the rest of the equations follow from definitions and algebra.

$$\begin{aligned}
E(X)E(Y) &= \sum_{i=1}^{k} x_i P(X = x_i) \sum_{j=1}^{m} y_j P(Y = y_j) \\
&= \sum_{i=1}^{k}\sum_{j=1}^{m} x_i y_j P(X = x_i) P(y = y_j) \\
&= \sum_{z:\ z \text{is a value of } XY} z \sum_{(i,j): x_i y_j = z} P(X = x_i)P(Y = y_j) \qquad (5.44) \\
&= \sum_{z:\ z \text{is a value of } XY} z \sum_{(i,j): x_i y_j = z} P((X = x_i) \wedge (Y = y_j)) \qquad (5.45) \\
&= \sum_{z:\ z \text{is a value of } XY} z P(XY = z) \\
&= E(XY).
\end{aligned}$$

■

Theorem 5.28 *If X and Y are independent random variables then*

$$V(X+Y) = V(X) + V(Y).$$

Proof: Using the definitions, algebra and linearity of expectation we have

$$\begin{aligned}
V(X+Y) &= E\left((X + Y - E(X+Y))^2\right) \\
&= E\left((X - E(X) + Y - E(Y))^2\right) \\
&= E\left(((X - E(X))^2 + 2(X - E(X))(Y - E(Y)) + (Y - E(Y))^2)\right) \\
&= E\left((X - E(X))^2\right) + 2E((X - E(X))(Y - E(Y))) + E\left((Y - E(Y))^2\right).
\end{aligned}$$

Now the first and last terms are just the definitions of $V(X)$ and $V(Y)$ respectively. Note also that if X and Y are independent and b and c are constants, then $X - b$ and $Y - c$ are independent (See Problem 8 at the end of this section.) Thus we can apply Lemma 5.27 to the middle term to obtain

$$= V(X) + 2E(X - E(X))E(Y - E(Y)) + V(Y).$$

Now we apply Equation 5.42 to the middle term to show that it is 0. This proves the theorem. ■

With this theorem, computing the variance for ten flips of a coin is easy; as usual we have the random variable X_i that is 1 or 0 depending on whether or not the coin comes up heads. We saw that the variance of X_i is $1/4$, so the variance for $X_1 + X_2 + \cdots + X_{10}$ is $10/4 = 2.5$.

Exercise 5.7-5 Find the variance for 100 flips of a coin and 400 flips of a coin.

Exercise 5.7-6 The variance in the previous problem grew by a factor of four when the number of trials grew by a factor of 4, while the spread we observed in our histograms grew by a factor of 2. Can you suggest a natural measure of spread that fixes this problem?

For Exercise 5.7-5 recall that the variance for one flip was $1/4$. Therefore the variance for 100 flips is 25 and the variance for 400 flips is 100. Since this measure grows linearly with the size, we can take its square root to give a measure of spread that grows with the square root of the quiz size, as our observed "spread" did in the histograms. Taking the square root actually makes intuitive sense, because it "corrects" for the fact that we were measuring expected squared spread rather than expected spread.

The square root of the variance of a random variable is called the *standard deviation* of the random variable and is denoted by σ, or $\sigma(X)$ when there is a chance for confusion as to what random variable we are discussing. Thus the standard deviation for 100 flips is 5 and for 400 flips is 10. Notice that in both the 100 flip case and the 400 flip case, the "spread" we observed in the histogram was ± 3 standard deviations from the expected value. What about for 25 flips? For 25 flips the standard deviation will be $5/2$, so ± 3 standard deviations from the expected value is a range of 15 points, again what we observed. For the test scores the variance is .16 for one question, so the standard deviation for 25 questions will be 2, giving us a range of 12 points. For 100 questions the standard deviation will be 4, and for 400 questions the standard deviation will be 8. Notice again how three standard deviations relate to the spread we see in the histograms.

Our observed relationship between the spread and the standard deviation is no accident. A consequence of a theorem of probability known as the central limit theorem is that the percentage of results within one standard deviation of the mean in a relatively large number of independent trials with two outcomes is about 68%; the percentage within two standard deviations of the mean is about 95.5%, and the percentage within three standard deviations of the mean is about 99.7%.

The central limit theorem tells us about the probability that the sum of independent random variables with the same distribution function is between two numbers. When the number of random variables we are adding is sufficiently large, the theorem tells us the approximate probability that the sum is between a and b standard deviations from its expected value. (For example if $a = -1.5$ and $b = 2$, the theorem tells us an approximate probability that the sum is between 1.5 standard deviations less than its expected value and 2 standard deviations more than its expected value.) This approximate value is $\frac{1}{\sqrt{2\pi}}\int_a^b e^{-x^2/2}\,dx$.[8] The distribution given by that multiple of the integral is called the *normal distribution*. Since many of the things we observe in nature can be thought of as the outcome of multistage processes, and the quantities we measure are often the result of adding some quantity at each stage, the central limit theorem "explains" why we should expect to see normal distributions for so many of the things we do measure. While weights can be thought of as the sum of the weight change due to eating and exercise each week, say, this is not a natural interpretation for blood pressures. Thus while we shouldn't be particularly surprised that weights are normally distributed, we don't have the same basis for predicting that blood pressures would be normally distributed[9], even though they are!

Exercise 5.7-7 If we want to be 95% sure that the number of heads in n flips of a coin is within $\pm 1\%$ of the expected value, how big does n have to be?

Exercise 5.7-8 What is the variance and standard deviation for the number of right answers for someone taking a 100 question short answer test where each answer is graded

[8] Still more precisely, if we let μ be the expected value of the random variable X_i and σ be its standard deviation (all X_i have the same expected value and standard distribution since they have the same distribution) and scale the sum of our random variables by $Z = \frac{X_1+X_2+\ldots.X_n-n\mu}{\sigma\sqrt{n}}$, then the probability that $a \le Z \le b$ is $\frac{1}{\sqrt{2\pi}}\int_a^b e^{-x^2/2}\,dx$.

[9] Actually, this is a matter of opinion. One might argue that blood pressures respond to a lot of little additive factors.

either correct or incorrect if the person knows 80% of the subject material for the test the test and answers correctly each question she knows? Should we be surprised if such a student scores 90 or above on the test?

Recall that for one flip of a coin the variance is $1/4$, so that for n flips it is $n/4$. Thus for n flips the standard deviation is $\sqrt{n}/2$. We expect that 95% of our outcomes will be within 2 standard deviations of the mean (people always round 95.5 to 95) so we are asking when two standard deviations are 1% of $n/2$. Thus we want an n such that $2\sqrt{n}/2 = .01(.5n)$, or such that $\sqrt{n} = 5 \cdot 10^{-3}n$, or $n = 25 \cdot 10^{-6}n^2$. This gives us $n = 10^6/25 = 40,000$.

For Exercise 5.7-8, the expected number of correct answers on any given question is .8. The variance for each answer is $.8(1-.8)^2 + .2(0-.8)^2 = .8 \cdot .04 + .2 \cdot .64 = .032 + .128 = .16$. Notice this is $.8 \cdot (1-.8)$. The total score is the sum of the random variables giving the number of points on each question, and assuming the questions are independent of each other, the variance of their sum is the sum of their variances, or 16. Thus the standard deviation is 4. Since 90% is 2.5 standard deviations above the expected value, the probability of getting that a score that far from the expected value is somewhere between .05 and .003 by the Central Limit Theorem. (In fact it is just a bit more than .01). Assuming that someone is just as likely to be 2.5 standard deviations below the expected score as above, which is not exactly right but close, we see that it is quite unlikely that someone who knows 80% of the material would score 90% or above on the test. Thus we should be surprised by such a score, and take the score as evidence that the student likely knows more than 80% of the material.

Coin flipping and test taking are two special cases of Bernoulli trials. With the same kind of computations we used for the test score random variable, we can prove the following.

Theorem 5.29 *In Bernoulli trials with probability p of success, the variance for one trial is $p(1-p)$ and for n trials is $np(1-p)$, so the standard deviation for n trials is $\sqrt{np(1-p)}$.*

Proof: You are asked to give the proof in Problem 7.■

Important Concepts, Formulas, and Theorems

1. *Histogram. Histograms* are graphs which show for for each integer value x of a random variable X a rectangle of width 1, centered at x, whose height (and thus area) is proportional to the probability $P(X = x)$. Histograms can be drawn with non-unit width rectangles. When people draw a rectangle with a base ranging from $x = a$ to $x = b$, the area of the rectangle is the probability that X is between a and b.

2. *Expected Value of a Constant.* If X is a random variable that always takes on the value c, then $E(X) = c$. In particular, $E(E(X)) = E(X)$.

3. *Variance.* We define the *variance* $V(X)$ of a random variable X as the expected value of $(X - E(X))^2$. We can also express this as a sum over the individual elements of the sample space S and get that $V(X) = E\left((X - E(X))^2\right) = \sum_{s:s\in S} P(s)(X(s) - E(X))^2$.

4. *Independent Random Variables.* We say random variables X and Y are *independent* when the event that X has value x is independent of the event that Y has value y, regardless of the choice of x and y.

5. *Expected Product of Independent Random Variables.* If X and Y are independent random variables on a sample space S, then $E(XY) = E(X)E(Y)$.

6. *Variance of Sum of Independent Random Variables.* If X and Y are independent random variables then $V(X + Y) = V(X) + V(Y)$.

7. *Standard deviation.* The square root of the variance of a random variable is called the *standard deviation* of the random variable and is denoted by σ, or $\sigma(X)$ when there is a chance for confusion as to what random variable we are discussing.

8. *Variance and Standard Deviation for Bernoulli Trials.* In Bernoulli trials with probability p of success, the variance for one trial is $p(1-p)$ and for n trials is $np(1-p)$, so the standard deviation for n trials is $\sqrt{np(1-p)}$.

9. *Central Limit Theorem.* The central limit theorem says that the sum of independent random variables with the same distribution function is approximated well as follows. The probability that the random variable is between a and b is an appropriately chosen multiple of $\int_a^b e^{-cx^2}\,dx$, for some constant c, when the number of random variables we are adding is sufficiently large. This implies that the probability that a sum of independent random variables is within one, two, or three standard deviations of its expected value is approximately .68, .955, and .997.

Problems

1. Suppose someone who knows 60% of the material covered in a chapter of a textbook is taking a five question objective (each answer is either right or wrong, not multiple choice or true-false) quiz. Let X be the random variable that for each possible quiz, gives the number of questions the student answers correctly. What is the expected value of the random variable $X - 3$? What is the expected value of $(X - 3)^2$? What is the variance of X?

2. In Problem 1 let X_i be the number of correct answers the student gets on question i, so that X_i is either zero or one. What is the expected value of X_i? What is the variance of X_i? How does the sum of the variances of X_1 through X_5 relate to the variance of X for Problem 1?

3. We have a dime and a fifty cent piece in a cup. We withdraw one coin. What is the expected amount of money we withdraw? What is the variance? Now we draw a second coin, without replacing the first. What is the expected amount of money we withdraw? What is the variance? Suppose instead we consider withdrawing two coins from the cup together. What is the expected amount of money we withdraw, and what is the variance? What does this example show about whether the variance of a sum of random variables is the sum of their variances.

4. If the quiz in Problem 1 has 100 questions, what is the expected number of right answers, the variance of the expected number of right answers, and the standard deviation of the number of right answers?

5. Estimate the probability that a person who knows 60% of the material gets a grade strictly between 50 and 70 in the test of Exercise 5.7-4

6. What is the variance in the number of right answers for someone who knows 80% of the material on which a 25 question quiz is based? What if the quiz has 100 questions? 400 questions? How can we "correct" these variances for the fact that the "spread" in the histogram for the number of right answers random variable only doubled when we multiplied the number of questions in a test by 4?

7. Prove Theorem 5.29.

8. Show that if X and Y are independent and b and c are constant, then $X - b$ and $Y - c$ are independent.

9. We have a nickel, dime and quarter in a cup. We withdraw two coins, first one and then the second, without replacement. What is the expected amount of money and variance for the first draw? For the second draw? For the sum of both draws?

10. Show that the variance for n independent trials with two outcomes and probability p of success is given by $np(1-p)$. What is the standard deviation? What are the corresponding values for the number of failures random variable?

11. What are the variance and standard deviation for the sum of the tops of n dice that we roll?

12. How many questions need to be on a short answer test for us to be 95% sure that someone who knows 80% of the course material gets a grade between 75% and 85%?

13. Is a score of 70% on a 100 question true-false test consistent with the hypothesis that the test taker was just guessing? What about a 10 question true-false test? (This is not a plug and chug problem; you have to come up with your own definition of "consistent with.")

14. Given a random variable X, how does the variance of cX relate to that of X?

15. Draw a graph of the equation $y = x(1-x)$ for x between 0 and 1. What is the maximum value of y? Why does this show that the variance (see Problem 10 in this section) of the "number of successes" random variable for n independent trials is less than or equal to $n/4$?

16. This problem develops an important law of probability known as *Chebyshev's law*. Suppose we are given a real number $r > 0$ and we want to estimate the probability that the difference $|X(x) - E(X)|$ of a random variable from its expected value is more than r.

    (a) Let $S = \{x_1, x_2, \ldots, x_n\}$ be the sample space, and let $E = \{x_1, x_2, \ldots, x_k\}$ be the set of all x such that $|X(x) - E(X)| > r$. By using the formula that defines $V(X)$, show that
    $$V(X) > \sum_{i=1}^{k} P(x_i)r^2 = P(E)r^2$$

    (b) Show that the probability that $|X(x) - E(X)| \geq r$ is no more than $V(X)/r^2$. This is called *Chebyshev's law*.

17. Use Problem 15 of this section to show that in n independent trials with probability p of success,
$$P\left(\left|\frac{\#\ \text{of successes} - np}{n}\right| \geq r\right) \leq \frac{1}{4nr^2}$$

18. This problem derives an intuitive law of probability known as the *law of large numbers* from Chebyshev's law. Informally, the law of large numbers says if you repeat an experiment many times, the fraction of the time that an event occurs is very likely to be close to the probability of the event. In particular, we shall prove that for any positive number s, no matter how small, by making the number n independent trials in a sequence of independent trials large enough, we can make the probability that the number X of successes is between $np - ns$ and $np + ns$ as close to 1 as we choose. For example, we can make the probability that the number of successes is within 1% (or 0.1 per cent) of the expected number as close to 1 as we wish.

    (a) Show that the probability that $|X(x) - np| \geq sn$ is no more than $p(1-p)/s^2n$.

    (b) Explain why this means that we can make the probability that $X(x)$ is between $np - sn$ and $np + sn$ as close to 1 as we want by making n large.

19. On a true-false test, the score is often computed by subtracting the number of wrong answers from the number of right ones and converting that number to a percentage of the number of questions. What is the expected score on a true-false test graded this way of someone who knows 80% of the material in a course? How does this scheme change the standard deviation in comparison with an objective test? What must you do to the number of questions to be able to be a certain percent sure that someone who knows 80% gets a grade within 5 points of the expected percentage score?

20. Another way to bound the deviance from the expectation is known as Markov's inequality. This inequality says that if X is a random variable taking only non-negative values, then, for any $k \geq 1$,

$$P(X > kE(X)) \leq \frac{1}{k}.$$

    Prove this inequality.

Chapter 6

Graphs

6.1 Graphs

In this chapter we introduce a fundamental structural idea of discrete mathematics, that of a graph. Many situations in the applications of discrete mathematics may be modeled by the use of a graph, and many algorithms have their most natural description in terms of graphs. It is for this reason that graphs are important to the computer scientist. Graph theory is an ideal subject for developing a deeper understanding of proof by induction because induction, especially strong induction, seems to enter into the majority of proofs in graph theory.

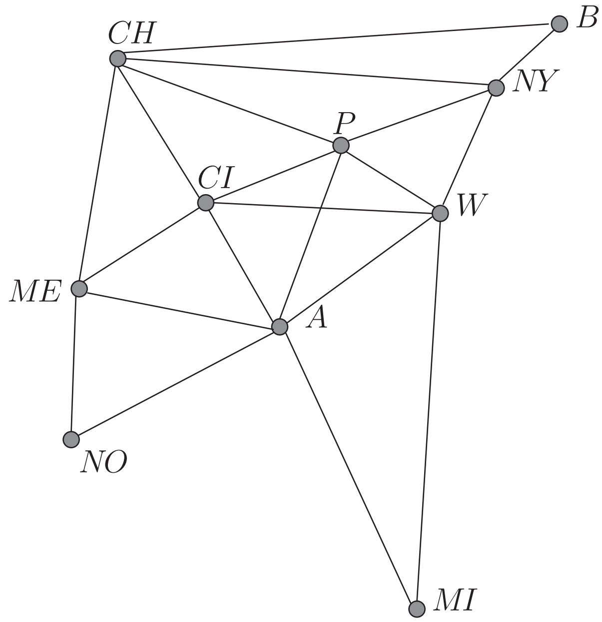
Exercise 6.1-1 In Figure 6.1, you see a stylized map of some cities in the eastern United States (Boston, New York, Pittsburgh, Cincinnati, Chicago, Memphis, New Orleans, Atlanta, Washington DC, and Miami). A company has major offices with data processing centers in each of these cities, and as its operations have grown, it has leased dedicated communication lines between certain pairs of these cities to allow for efficient communication among the computer systems in the various cities. Each grey dot in the figure stands for a data center, and each line in the figure stands for a dedicated communication link. What is the minimum number of links that could be used in sending a message from B (Boston) to NO (New Orleans)? Give a route with this number of links.

Exercise 6.1-2 Which city or cities has or have the most communication links emanating from them?

Exercise 6.1-3 What is the total number of communication links in the figure?

The picture in Figure 6.1 is a drawing of what we call a "graph". A **graph** consists of a set of *vertices* and a set of *edges* with the property that each edge has two (not necessarily different) vertices associated with it and called its *endpoints*. We say the edge *joins* the endpoints, and we say two endpoints are *adjacent* if they are joined by an edge. When a vertex is an endpoint of an edge, we say the edge and the vertex are *incident*. Several more examples of graphs are given in Figure 6.2. To *draw* a graph, we draw a point (in our case a grey circle) in the plane for each vertex, and then for each edge we draw a (possibly curved) line between the points that correspond to the endpoints of the edge. The only vertices that may be touched by the line

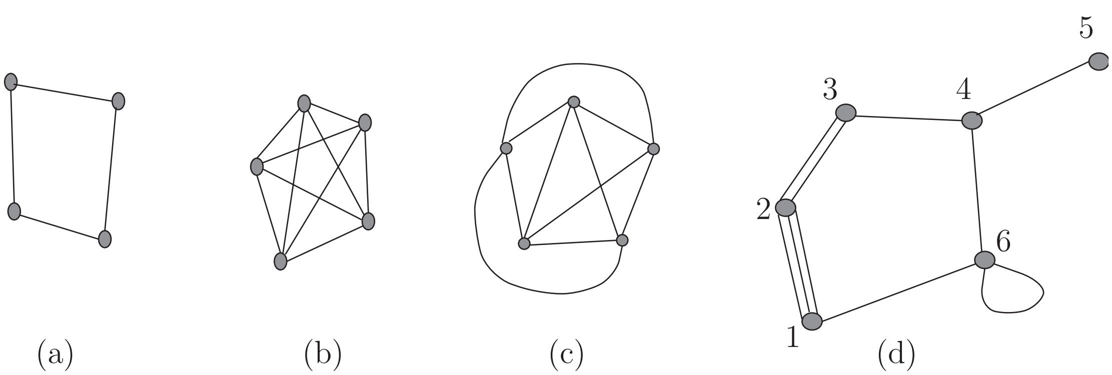
Figure 6.1: A stylized map of some eastern US cities.



representing an edge are the endpoints of the edge. Notice that in graph (d) of Figure 6.2 we have three edges joining the vertices marked 1 and 2 and two edges joining the vertices marked 2 and 3. We also have one edge that joins the vertex marked 6 to itself. This edge has two identical endpoints. The graph in Figure 6.1 and the first three graphs in Figure 6.2 are called simple graphs. A *simple graph* is one that has at most one edge joining each pair of distinct vertices, and no edges joining a vertex to itself.[1] You'll note in Figure 6.2 that we sometimes label the vertices of the graph and we sometimes don't. We label the vertices when we want to give them meaning,

[1]The terminology of graph theory has not yet been standardized, because it is a relatively young subject. The terminology we are using here is the most popular terminology in computer science, but some graph theorists would reserve the word graph for what we have just called a simple graph and would use the word multigraph for what we called a graph.

Figure 6.2: Some examples of graphs



as in Figure 6.1 or when we know we will want to refer to them as in graph (d) of Figure 6.2. We say that graph (d) in Figure 6.2 has a "loop" at vertex 6 and multiple edges joining vertices 1 and 2 and vertices 2 and 3. More precisely, an edge that joins a vertex to itself is called a *loop* and we say we have *multiple edges* between vertices x and y if there is more than one edge joining x and y. If there is an edge from vertex x to vertex y in a simple graph, we denote it by $\{x, y\}$. Thus $\{P, W\}$ denotes the edge between Pittsburgh and Washington in Figure 6.1 Sometimes it will be helpful to have a symbol to stand for a graph. We use the phrase "Let $G = (V, E)$" as a shorthand for "Let G stand for a graph with vertex set V and edge set E."

The drawings in parts (b) and (c) of Figure 6.2 are different drawings of the same graph. The graph consists of five vertices and one edge between each pair of distinct vertices. It is called the complete graph on five vertices and is denoted by K_5. In general, a *complete graph* on n vertices is a graph with n vertices that has an edge between each two of the vertices. We use K_n to stand for a complete graph on n vertices. These two drawings are intended to illustrate that there are many different ways we can draw a given graph. The two drawings illustrate two different ideas. Drawing (b) illustrates the fact that each vertex is adjacent to each other vertex and suggests that there is a high degree of symmetry. Drawing (c) illustrates the fact that it is possible to draw the graph so that only one pair of edges crosses; other than that the only places where edges come together are at their endpoints. In fact, it is impossible to draw K_5 so that no edges cross, a fact that we shall explain later in this chapter.

In Exercise 6.1-1 the links referred to are edges of the graph and the cities are the vertices of the graph. It is possible to get from the vertex for Boston to the vertex for New Orleans by using three communication links, namely the edge from Boston to Chicago, the edge from Chicago to Memphis, and the edge from Memphis to New Orleans. A **path** in a graph is an alternating sequence of vertices and edges such that

- it starts and ends with a vertex, and
- each edge joins the vertex before it in the sequence to the vertex after it in the sequence.[2]

If a is the first vertex in the path and b is the last vertex in the path, then we say the path is a path from a to b. Thus the path we found from Boston to New Orleans is $B\{B, CH\}CH\{CH, ME\}, ME\{ME, NO\}NO$. Because the graph is simple, we can also use the shorter notation B, CH, ME, NO to describe the same path, because there is exactly one edge between successive vertices in this list. The *length* of a path is the number of edges it has, so our path from Boston to New Orleans has length 3. The length of a shortest path between two vertices in a graph is called the *distance* between them. Thus the distance from Boston to New Orleans in the graph of Figure 6.1 is three. By inspecting the map we see that there is no shorter path from Boston to New Orleans. Notice that no vertex or edge is repeated on our path from Boston to New Orleans. A path is called a **simple path** if it has no repeated vertices or edges.[3]

The degree of a vertex

In Exercise 6.1-2, the city with the most communication links is Atlanta (A). We say the vertex A has "degree" 6 because 6 edges emanate from it. More generally the *degree* of a vertex in a

[2] Again, the terminology we are using here is the most popular terminology in computer science, but what we just defined as a path would be called a walk by most graph theorists.

[3] Most graph theorists reserve the word path for what we are calling a simple path, but again we are using the language most popular in computer science.

graph is the number of times it is incident with edges of the graph; that is, the degree of a vertex x is the number of edges from x to other vertices plus twice the number of loops at vertex x. In graph (d) of Figure 6.2 vertex 2 has degree 5, and vertex 6 has degree 4. In a graph like the one in Figure 6.1, it is somewhat difficult to count the edges just because you can forget which ones you've counted and which ones you haven't.

Exercise 6.1-4 Is there a relationship between the number of edges in a graph and the degrees of the vertices? If so, find it. Hint: computing degrees of vertices and number of edges in some relatively small examples of graphs should help you discover a formula. To find one proof, imagine a wild west movie in which the villain is hiding under the front porch of a cabin. A posse rides up and is talking to the owner of the cabin, and the bad guy can just barely look out from underneath the porch and count the horses hoofs. If he counts the hooves accurately, what can he do to figure out the number of horses, and thus presumably the size of the posse?

In Exercise 6.1-4, examples such as those in Figure 6.2 convince us that the sum of the degrees of the vertices is twice the number of edges. How can we prove this? One way is to count the total number of incidences between vertices and edges (similar to counting the horses hooves in the hint). Each edge has exactly two incidences, so the total number of incidences is twice the number of edges. But the degree of a vertex is the number of incidences it has, so the sum of the degrees of the vertices is also the total number of of incidences. Therefore the sum of the degrees of the vertices of a graph is twice the number of edges. Thus to compute the number of edges of a graph, we can sum the degrees of the vertices and divide by two. (In the case of the hint, the horses correspond to edges and the hooves to endpoints.) There is another proof of this result that uses induction.

Theorem 6.1 *Suppose a graph has a finite number of edges. Then the sum of the degrees of the vertices is twice the number of edges.*

Proof: We induct on the number of edges of the graph. If a graph has no edges, then each vertex has degree zero and the sum of the degrees is zero, which is twice the number of edges. Now suppose $e > 0$ and the theorem is true whenever a graph has fewer than e edges. Let G be a graph with e edges and let ϵ be an edge of G.[4] Let G' be the graph (on the same vertex set as G) we get by deleting ϵ from the edge set E of G. Then G has $e-1$ edges, and so by our inductive hypothesis, the sum of the degrees of the vertices of G' is twice $e-1$. Now there are two possible cases. Either e was a loop, in which case one vertex of G' has degree two less in G' than it has in G. Otherwise e has two distinct endpoints, in which case exactly two vertices of G' have degree one less than their degree in G. Thus in both cases the sum of the degrees of the vertices in G' is two less than the sum of the degrees of the vertices in G, so the sum of the degrees of the vertices in G is $(2e-2)+2 = 2e$. Thus the truth of the theorem for graphs with $e-1$ edges implies the truth of the theorem for graphs with e edges. Therefore, by the principle of mathematical induction, the theorem is true for a graph with any finite number of edges. ■

There are a couple instructive points in the proof of the theorem. First, since it wasn't clear from the outset whether we would need to use strong or weak induction, we made the inductive

[4]Since it is very handy to have e stand for the number of edges of a graph, we will use Greek letters such as epsilon (ϵ) to stand for edges of a graph. It is also handy to use v to stand for the number of vertices of a graph, so we use other letters near the end of the alphabet, such as w, x, y,and z to stand for vertices.

hypothesis we would normally make for strong induction. However in the course of the proof, we saw that we only needed to use weak induction, so that is how we wrote our conclusion. This is not a mistake, because we used our inductive hypothesis correctly. We just didn't need to use it for every possible value it covered.

Second, instead of saying that we would take a graph with $e-1$ edges and add an edge to get a graph with e edges, we said that we would take a graph with e edges and remove an edge to get a graph with $e-1$ edges. This is because we need to prove that the result holds for *every* graph with e edges. By using the second approach we avoided the need to say that "every graph with e edges may be built up from a graph with $e-1$ edges by adding an edge," because in the second approach we started with an arbitrary graph on e edges. In the first approach, we would have proved that the theorem was true for all graphs that could be built from an $e-1$ edge graph by adding an edge, and we would have had to explicitly say that every graph with e edges could be built in this way.

In Exercise 3 the sum of the degrees of the vertices is (working from left to right)

$$2+4+5+6+5+2+5+4+2=40,$$

and so the graph has 20 edges.

Connectivity

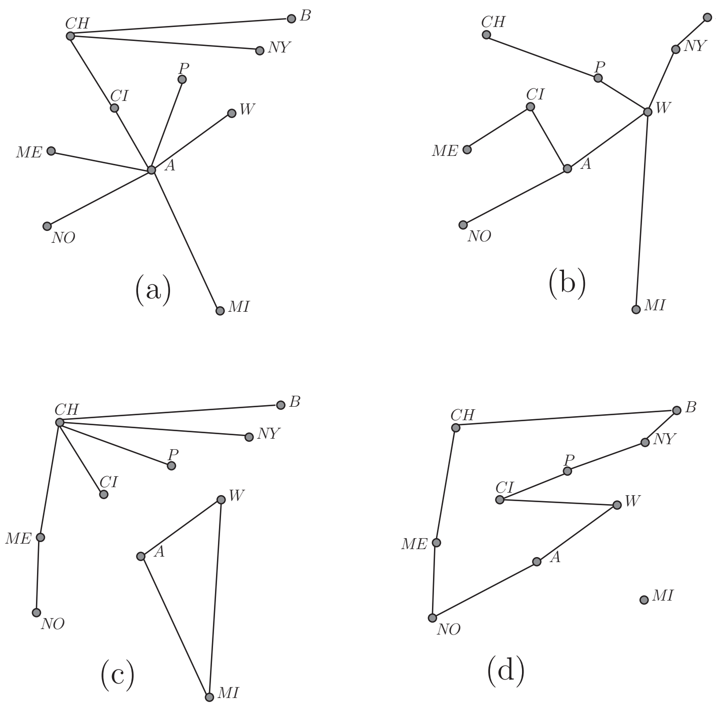
All of the examples we have seen so far have a property that is not common to all graphs, namely that there is a path from every vertex to every other vertex.

Exercise 6.1-5 The company with the computer network in Figure 6.1 needs to reduce its expenses. It is currently leasing each of the communication lines shown in the Figure. Since it can send information from one city to another through one or more intermediate cities, it decides to only lease the minimum number of communication lines it needs to be able to send a message from any city to any other city by using any number of intermediate cities. What is the minimum number of lines it needs to lease? Give two examples of subsets of the edge set with this number of edges that will allow communication between any two cities and two examples of a subset of the edge set with this number of edges that will not allow communication between any two cities.

Some experimentation with the graph convinces us that if we keep eight or fewer edges, there is no way we can communicate among the cities (we will explain this more precisely later on), but that there are quite a few sets of nine edges that suffice for communication among all the cities. In Figure 6.3 we show two sets of nine edges each that allow us to communicate among all the cities and two sets of nine edges that do not allow us to communicate among all the cities.

Notice that in graphs (a) and (b) it is possible to get from any vertex to any other vertex by a path. A graph is called *connected* there is a path between each two vertices of the graph. Notice that in graph (c) it is not possible to find a path from Atlanta to Boston, for example, and in graph (d) it is not possible to find a path from Miami to any of the other vertices. Thus these graphs are not connected; we call them disconnected. In graph (d) we say that Miami is an *isolated vertex*.

Figure 6.3: Selecting nine edges from the stylized map of some eastern US cities.



We say two vertices are *connected* if there is a path between them, so a graph is connected if each two of its vertices are connected. Thus in Graph (c) the vertices for Boston and New Orleans are connected. The relationship of being connected is an equivalence relation (in the sense of Section 1.4). To show this we would have to show that this relationship divides the set of vertices up into mutually exclusive classes; that is, that it partitions the vertices of the graph. The class containing Boston, for example is all vertices connected to Boston. If two vertices are in that set, they both have paths to Boston, so there is a path between them using Boston as an intermediate vertex. If a vertex x is in the set containing Boston and another vertex y is not, then they cannot be connected or else the path from y to x and then on to Boston would connect y to Boston, which would mean y was in the class containing Boston after all. Thus the relation of being connected partitions the vertex set of the graph into disjoint classes, so it is an equivalence relation. Though we made this argument with respect to the vertex Boston in the specific case of graph (c) of Figure 6.3, it is a perfectly general argument that applies to arbitrary vertices in arbitrary graphs. We call the equivalence relation of "being connected to" the *connectivity* relation. There can be no edge of a graph between two vertices in different equivalence classes of the connectivity relation because then everything in one class would be connected to everything in the other class, so the two classes would have to be the same. Thus we also end up with a partition of the edges into disjoint sets. If a graph has edge set E, and C is an equivalence class of the connectivity relation, then we use $E(C)$ to denote the set of edges whose endpoints are both in C. Since no edge connects vertices in different equivalence classes, each edge must be in some set $E(C)$. The graph consisting of an equivalence class C of the connectivity relation together with the edges $E(C)$ is called a *connected component* of our original graph. From now on our emphasis will be on connected components rather than on equivalence classes of the connectivity relation. Notice that graphs (c) and (d) of Figure 6.3 each have two connected components. In graph (c) the vertex sets of the connected components are $\{NO, ME, CH, CI, P, NY, B\}$ and $\{A, W, MI\}$. In graph (d) the connected components are $\{NO, ME, CH, B, NY, P, CI, W, A\}$ and $\{MI\}$. Two other examples of graphs with multiple connected components are shown in Figure 6.4.

Figure 6.4: A simple graph G with three connected components and a graph H with four connected components.

Cycles

In graphs (c) and (d) of Figure 6.3 we see a feature that we don't see in graphs (a) and (b), namely a path that leads from a vertex back to itself. A path that starts and ends at the same vertex is called a *closed path*. A closed path with at least one edge is called a *cycle* if, except for the last vertex, all of its vertices are different. The closed paths we see in graphs (c) and (d) of Figure 6.3 are cycles. Not only do we say that $\{NO, ME, CH, B, NY, P, CI, W, A, NO\}$ is a cycle in in graph (d) of Figure 6.3, but we also say it is a cycle in the graph of Figure 6.1. The way we distinguish between these situations is to say the cycle $\{NO, ME, CH, B, NY, P, CI, W, A, NO\}$ is an induced cycle in Figure 6.3 but not in Figure 6.1. More generally, a graph H is called a *subgraph* of the graph G if all the vertices and edges of H are vertices and edges of G. We call H an *induced subgraph* of G if every vertex of H is a vertex of G, and every edge of G connecting vertices of H is an edge of H. Thus the first graph of Figure 6.4 has an induced K_4 and an induced cycle on three vertices.

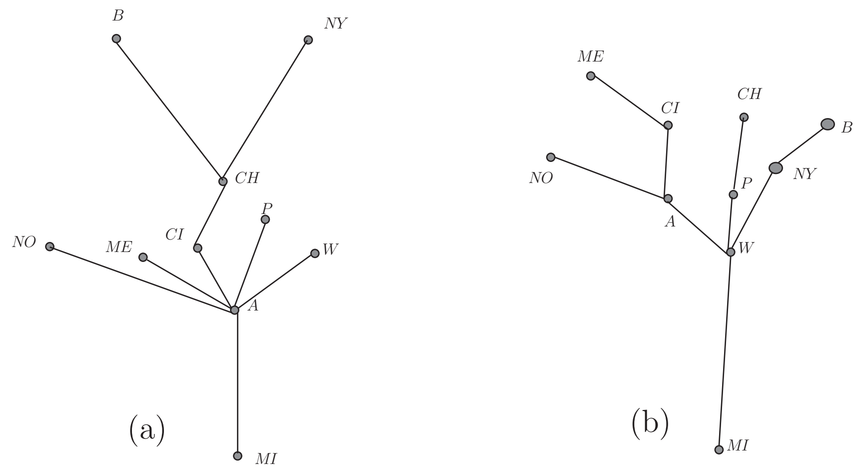
We don't normally distinguish which point on a cycle really is the starting point; for example we consider the cycle $\{A, W, MI, A\}$ to be the same as the cycle $\{W, MI, A, W\}$. Notice that there are cycles with one edge and cycles with two edges in the second graph of Figure 6.4. We call a graph G a *cycle* on n vertices or an n-cycle and denote it by C_n if it has a cycle that contains all the vertices and edges of G and a *path* on n vertices and denote it by P_n if it has a path that contains all the vertices and edges of G. Thus drawing (a) of Figure 6.2 is a drawing of C_4. The second graph of Figure 6.4 has an induced P_3 and an induced C_2 as subgraphs.

Trees

The graphs in parts (a) and (b) of Figure 6.3 are called trees. We have redrawn them slightly in Figure 6.5 so that you can see why they are called trees. We've said these two graphs are called trees, but we haven't given a definition of trees. In the examples in Figure 6.3, the graphs we have called trees are connected and have no cycles.

Definition 6.1 *A connected graph with no cycles is called a tree.*

Figure 6.5: A visual explanation of the name tree.



Other Properties of Trees

In coming to our definition of a tree, we left out a lot of other properties of trees we could have discovered by a further analysis of Figure 6.3

Exercise 6.1-6 Given two vertices in a tree, how many distinct simple paths can we find between the two vertices?

Exercise 6.1-7 Is it possible to delete an edge from a tree and have it remain connected?

Exercise 6.1-8 If $G = (V, E)$ is a graph and we add an edge that joins vertices of V, what can happen to the number of connected components?

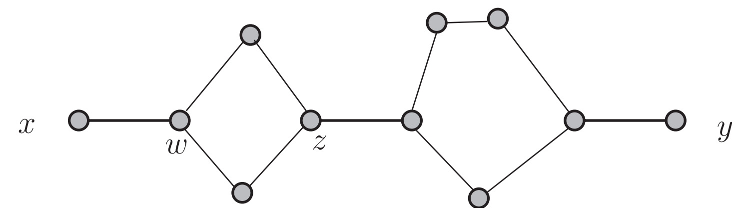
Exercise 6.1-9 How many edges does a tree with v vertices have?

Exercise 6.1-10 Does every tree have a vertex of degree 1? If the answer is yes, explain why. If the answer is no, try to find additional conditions that will guarantee that a tree satisfying these conditions has a vertex of degree 1.

For Exercise 6.1-6, suppose we had two distinct paths from a vertex x to a vertex y. They begin with the same vertex x and might have some more edges in common as in Figure 6.6. Let w be the last vertex after (or including) x the paths share before they become different. The paths must come together again at y, but they might come together earlier. Let z be the first vertex the paths have in common after w. Then there are two paths from w to z that have only w and z in common. Taking one of these paths from w to z and the other from z to w gives us a cycle, and so the graph is not a tree. We have shown that if a graph has two distinct paths from x to y, then it is not a tree. By contrapositive inference, then, if a graph is a tree, it does not have two distinct paths between two vertices x and y. We state this result as a theorem.

Theorem 6.2 *There is exactly one path between each two vertices in a tree.*

Figure 6.6: A graph with multiple paths from x to y.



Proof: By the definition of a tree, there is at least one path between each two vertices. By our argument above, there is at most one path between each two vertices. Thus there is exactly one path. ■

For Exercise 6.1-7, note that if ϵ is an edge from x to y, then x, ϵ, y is the unique path from x to y in the tree. Suppose we delete ϵ from the edge set of the tree. If there were still a path from x to y in the resulting graph, it would also be a path from x to y in the tree, which would contradict Theorem 6.2. Thus the only possibility is that there is no path between x and y in the resulting graph, so it is not connected and is therefore not a tree.

For Exercise 6.1-8, if the endpoints are in the same connected component, then the number of connected components won't change. If the endpoints of the edge are in different connected components, then the number of connected components can go down by one. Since an edge has two endpoints, it is impossible for the number of connected components to go down by more than one when we add an edge. This paragraph and the previous one lead us to the following useful lemma.

Lemma 6.3 *Removing one edge from the edge set of a tree gives a graph with two connected components, each of which is a tree.*

Proof: Suppose as before the lemma that ϵ is an edge from x to y. We have seen that the graph G we get by deleting ϵ from the edge set of the tree is not connected, so it has at least two connected components. But adding the edge back in can only reduce the number of connected compponents by one. Therefore G has exactly two connected components. Since neither has any cycles, both are trees. ■

In Exercise 6.1-9, our trees with ten vertices had nine edges. If we draw a tree on two vertices it will have one edge; if we draw a tree on three vertices it will have two edges. There are two different looking trees on four vertices as shown in Figure 6.7, and each has three edges. On the

Figure 6.7: Two trees on four vertices.

basis of these examples we conjecture that a tree on n vertices has $n - 1$ edges. One approach to proving this is to try to use induction. To do so, we have to see how to build up every tree from smaller trees or how to take a tree and break it into smaller ones. Then in either case we have to figure out how use the truth of our conjecture for the smaller trees to imply its truth for the larger trees. A mistake that people often make at this stage is to assume that every tree can be built from smaller ones by adding a vertex of degree 1. While that is true for finite trees with more than one vertex (which is the point of Exercise 6.1-10), we haven't proved it yet, so we can't yet use it in proofs of other theorems. Another approach to using induction is to ask whether there is a natural way to break a tree into two smaller trees. There is: we just showed in Lemma 6.3 that if you remove an edge ϵ from the edge set of a tree, you get two connected components that are trees. We may assume inductively that the number of edges of each of these trees is one less than its number of vertices. Thus if the graph with these two connected components has v vertices, then it has $v-2$ edges. Adding ϵ back in gives us a graph with $v-1$ edges, so except for the fact that we have not done a base case, we have proved the following theorem.

Theorem 6.4 *For all integers $v \geq 1$, a tree with v vertices has $v-1$ edges.*

Proof: If a tree has one vertex, it can have no edges, for any edge would have to connect that vertex to itself and would thus give a cycle. A tree with two or more vertices must have an edge in order to be connected. We have shown before the statement of the theorem how to use the deletion of an edge to complete an inductive proof that a tree with v vertices has $v-1$ edges, and so for all $v \geq 1$, a tree with v vertices has $v-1$ edges. ■

Finally, for Exercise 6.1-10 we can now give a contrapositive argument to show that a finite tree with more than one vertex has a vertex of degree one. Suppose instead that G is a graph that is connected and all vertices of G have degree two or more. Then the sum of the degrees of the vertices is at least 2v, and so by Theorem 6.1 the number of edges is at least v. Therefore by Theorem 6.4 G is not a tree. Then by contrapositive inference, if T is a tree, then T must have at least one vertex of degree one. This corollary to Theorem 6.4 is so useful that we state it formally.

Corollary 6.5 *A finite tree with more than one vertex has at least one vertex of degree one.*

Important Concepts, Formulas, and Theorems

1. *Graph.* A *graph* consists of a set of *vertices* and a set of *edges* with the property that each edge has two (not necessarily different) vertices associated with it and called its *endpoints*.

2. *Edge; Adjacent.* We say an edge in a graph *joins* its endpoints, and we say two endpoints are *adjacent* if they are joined by an edge.

3. *Incident.* When a vertex is an endpoint of an edge, we say the edge and the vertex are *incident*.

4. *Drawing of a Graph.* To *draw* a graph, we draw a point in the plane for each vertex, and then for each edge we draw a (possibly curved) line between the points that correspond to the endpoints of the edge. Lines that correspond to edges may only touch the vertices that are their endpoints.

5. *Simple Graph.* A *simple graph* is one that has at most one edge joining each pair of distinct vertices, and no edges joining a vertex to itself.

6. *Length, Distance.* The *length* of a path is the number of edges. The *distance* between two vertices in a graph is the length of a shortest path between them.

7. *Loop; Multiple Edges.* An edge that joins a vertex to itself is called a loop and we say we have multiple edges between vertices x and y if there is more than one edge joining x and y.

8. *Notation for a Graph.* We use the phrase "Let $G = (V, E)$" as a shorthand for "Let G stand for a graph with vertex set V and edge set E."

9. *Notation for Edges.* In a simple graph we use the notation $\{x, y\}$ for an edge from x to y. In any graph, when we want to use a letter to denote an edge we use a Greek letter like ϵ so that we can save e to stand for the number of edges of the graph.

10. *Complete Graph on n vertices.* A *complete graph* on n vertices is a graph with n vertices that has an edge between each two of the vertices. We use K_n to stand for a complete graph on n vertices.

11. *Path.* We call an alternating sequence of vertices and edges in a graph a *path* if it starts and ends with a vertex, and each edge joins the vertex before it in the sequence to the vertex after it in the sequence.

12. *Simple Path.* A path is called a *simple path* if it has no repeated vertices or edges.

13. *Degree of a Vertex.* The *degree* of a vertex in a graph is the number of times it is incident with edges of the graph; that is, the degree of a vertex x is the number of edges from x to other vertices plus twice the number of loops at vertex x.

14. *Sum of Degrees of Vertices.* The sum of the degrees of the vertices in a graph with a finite number of edges is twice the number of edges.

15. *Connected.* A graph is called *connected* if there is a path between each two vertices of the graph. We say two vertices are *connected* if there is a path between them, so a graph is connected if each two of its vertices are connected. The relationship of being connected is an equivalence relation on the vertices of a graph.

16. *Connected Component.* If C is a subset of the vertex set of a graph, we use $E(C)$ to stand for the set of all edges *both* of whose endpoints are in C. The graph consisting of an equivalence class C of the connectivity relation together with the edges $E(C)$ is called a *connected component* of our original graph.

17. *Closed Path.* A path that starts and ends at the same vertex is called a *closed path.*

18. *Cycle.* A closed path with at least one edge is called a *cycle* if, except for the last vertex, all of its vertices are different.

19. *Tree.* A connected graph with no cycles is called a tree.

20. *Important Properties of Trees.*

    (a) There is a unique path between each two vertices in a tree.

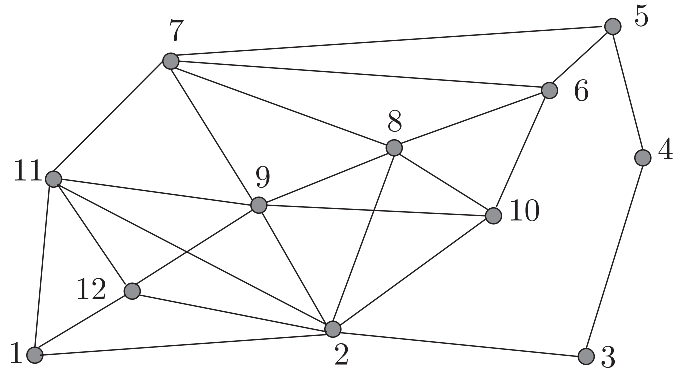
    (b) A tree on v vertices has $v - 1$ edges.

    (c) Every finite tree with at least two vertices has a vertex of degree one.

Problems

1. Find the shortest path you can from vertex 1 to vertex 5 in Figure 6.8.

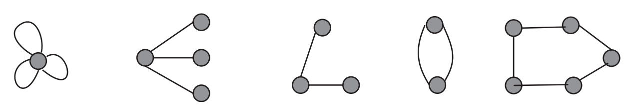
Figure 6.8: A graph.



2. Find the longest simple path you can from vertex 1 to vertex 5 in Figure 6.8.

3. Find the vertex of largest degree in Figure 6.8. What is it's degree?

Figure 6.9: A graph with a number of connected components.



4. How many connected components does the graph in Figure 6.9 have?

5. Find all induced cycles in the graph of Figure 6.9.

6. What is the size of the largest induced K_n in Figure 6.9?

7. Find the largest induced K_n (in words, the largest complete subgraph) you can in Figure 6.8.

8. Find the size of the largest induced P_n in the graph in Figure 6.9.

9. A graph with no cycles is called a *forest*. Show that if a forest has v vertices, e edges, and c connected components, then $v = e + c$.

10. What can you say about a five vertex simple graph in which every vertex has degree four?

11. Find a drawing of K_6 in which only three pairs of edges cross.

12. Either prove true or find a counter-example. A graph is a tree if there is one and only one simple path between each pair of vertices.

13. Is there some number m such that if a graph with v vertices is connected and has m edges, then it is a tree? If so, what is m in terms of v?

14. Is there some number m such that a graph on n vertices is a tree if and only if it has m edges and has no cycles.

15. Suppose that a graph G is connected, but for each edge, deleting that edge leaves a disconnected graph. What can you say about G? Prove it.

16. Show that each tree with four vertices can be drawn with one of the two drawings in Figure 6.7.

17. Draw the minimum number of drawings of trees you can so that each tree with five vertices has one of those drawings. Explain why you have drawn all possible trees.

18. Draw the minimum number of drawings of trees you can so that each tree with six vertices is represented by exactly one of those drawings. Explaining why you have drawn all possible drawings is optional.

19. Find the longest induced cycle you can in Figure 6.8.

6.2 Spanning Trees and Rooted Trees

Spanning Trees

We introduced trees with the example of choosing a minimum-sized set of edges that would connect all the vertices in the graph of Figure 6.1. That led us to discuss trees. In fact the kinds of trees that solve our original problem have a special name. A tree whose edge set is a subset of the edge set of the graph G is called a *spanning tree* of G if the tree has exactly the same vertex set as G. Thus the graphs (a) and (b) of Figure 6.3 are spanning trees of the graph of Figure 6.1.

Exercise 6.2-1 Does every connected graph have a spanning tree? Either give a proof or a counter-example.

Exercise 6.2-2 Give an algorithm that determines whether a graph has a spanning tree, finds such a tree if it exists, and takes time bounded above by a polynomial in v and e, where v is the number of vertices, and e is the number of edges.

For Exercise 6.2-1, if the graph has no cycles but is connected, it is a tree, and thus is its own spanning tree. This makes a good base step for a proof by induction on the number of cycles of the graph that every connected graph has a spanning tree. Let $c > 0$ and suppose inductively that when a connected graph has fewer than c cycles, then the graph has a spanning tree. Suppose that G is a graph with c cycles. Choose a cycle of G and choose an edge of that cycle. Deleting that edge (but not its endpoints) reduces the number of cycles by at least one, and so our inductive hypothesis implies that the resulting graph has a spanning tree. But then that spanning tree is also a spanning tree of G. Therefore by the principle of mathematical induction, every finite connected graph has a spanning tree. We have proved the following theorem.

Theorem 6.6 *Each finite connected graph has a spanning tree.*

Proof: The proof is given before the statement of the theorem.■

In Exercise 6.2-2, we want an algorithm for determining whether a graph has a spanning tree. One natural approach would be to convert the inductive proof of Theorem 6.6 into a recursive algorithm. Doing it in the obvious way, however, would mean that we would have to search for cycles in our graph. A natural way to look for a cycle is to look at each subset of the vertex set and see if that subset is a cycle of the graph. Since there are 2^v subsets of the vertex set, we could not guarantee that an algorithm that works in this way would find a spanning tree in time which is big Oh of a polynomial in v and e. In an algorithms course you will learn a much faster (and much more sophisticated) way to implement this approach. We will use another approach, describing a quite general algorithm which we can then specialize in several different ways for different purposes.

The idea of the algorithm is to build up, one vertex at a time, a tree that is a subgraph (not necessarily an induced subgraph) of the graph $G = (V, E)$. (A subgraph of G that is a tree is called a *subtree* of G.) We start with some vertex, say x_0. If there are no edges leaving the vertex and the graph has more than one vertex, we know the graph is not connected and we therefore don't have a spanning tree. Otherwise, we can choose an edge ϵ_1 that connects x_0 to another vertex x_1. Thus $\{x_0, x_1\}$ is the vertex set of a subtree of G. Now if there are no edges that connect some vertex in the set $\{x_0, x_1\}$ to a vertex not in that set, then $\{x_0, x_1\}$ is a connected component of G. In this case, either G is not connected and has no spanning tree, or it just has two vertices and we have a spanning tree. However if there is an edge that connects some vertex in the set $\{x_0, x_1\}$ to a vertex not in that set, we can use this edge to continue building a tree. This suggests an inductive approach to building up the vertex set S of a subtree of our graph one vertex at a time. For the base case of the algorithm, we let $S = \{x_0\}$. For the inductive step, given S, we choose an edge ϵ that leads from a vertex in S to a vertex in $V - S$ (provided such an edge exists) and add it to the edge set E' of the subtree. If no such edge exists, we stop. If $V = S$ when we stop then E' is the edge set of a spanning tree. (We can prove inductively that E' is the edge set of a tree on S, because adding a vertex of degree one to a tree gives a tree.) If $V \neq S$ when we stop, G is not connected and does not have a spanning tree.

To describe the algorithm a bit more precisely, we give pseudocode.

Spantree(V,E)
// Assume that V is an array that lists the vertex set of the graph.
// Assume that E is an array with $|V|$ entries, and entry i of E is the set of
// edges incident with the vertex in position i of V.
(1) $i = 0$;
(2) Choose a vertex x_0 in V.
(3) $S = \{x_0\}$
(4) While there is an edge from a vertex in S to a vertex not in S
(5)   i=i+1
(6)   Choose an edge ϵ_i from a vertex y in S to a vertex x_i not in S
(7) $S = S \cup \{x_i\}$
(8) $E' = E' \cup \epsilon_i$
(9) If $i = |V| - 1$
(10)   return E'
(11) Else
(12)   Print "The graph is not connected."

The way in which the vertex x_i and the edge ϵ_i are chosen was deliberately left vague because there are several different ways to specify x_i and ϵ_i that accomplish several different purposes. However, with some natural assumptions, we can still give a big Oh bound on how long the algorithm takes. Presumably we will need to consider at most all v vertices of the graph in order to choose x_i, and so assuming we decide whether or not to use a vertex in constant time, this step of the algorithm will take $O(v)$ time. Presumably we will need to consider at most all e edges of our graph in order to choose ϵ_i, and so assuming we decide whether or not to use an edge in constant time, this step of the algorithm takes at most $O(e)$ time. Given the generality of the condition of the while loop that begins in line 4, determining whether that condition is true might also take $O(e)$ time. Since we repeat the While loop at most v times, all executions of the While loop should take at most $O(ve)$ time. Since line 9 requires us to compute $|V|$, it takes $O(v)$ steps, and all the other lines take constant time. Thus, with the assumptions we have made, the algorithm takes $O(ve + v + e) = O(ve)$ time.

Breadth First Search

Notice that algorithm Spantree will continue as long as a vertex in S is connected to a vertex not in S. Thus when it stops, S will be the vertex set of a connected component of the graph and E' will be the edge set of a spanning tree of this connected component. This suggests that one use that we might make of algorithm Spantree is to find connected components of graphs. If we want the connected component containing a specific vertex x, then we make this choice of x_0 in Line 2. Suppose this is our goal for the algorithm, and suppose that we also want to make the algorithm run as quickly as possible. We could guarantee a faster running time if we could arrange our choice of ϵ_i so that we examined each edge no more than some constant number of times between the start and the end of the algorithm. One way to achieve this is to first use all edges incident with x_0 as ϵ_is, then consider all edges incident with x_1, using them as ϵ_i if we can, and so on.

We can describe this process inductively. We begin by choosing a vertex x_0 and putting vertex x_0 in S and (except for loops or multiple edges) all edges incident with x_0 in E'. As we put edges into E', we number them, starting with ϵ_1. This creates a list $\epsilon_1, \epsilon_2, \ldots$ of edges. When we add edge ϵ_i to the tree, one of its two vertices is not yet numbered. We number it as x_i. Then given vertices 0 through i, all of whose incident edges we have examined and either accepted or (permanently) rejected as a member of E' (or more symbolically, as an ϵ_j), we examine the edges leaving vertex $i+1$. For each of these edges that is incident with a vertex not already in S, we add the edge and that vertex to the tree, numbering the edges and vertices as described above. Otherwise we reject that edge. Eventually we reach a point where we have examined all the edges leaving all the vertices in S, and we stop.

To give a pseudocode description of the algorithm, we assume that we are given an array V that contains the names of the vertices. There are a number of ways to keep track of the edge set of a graph in a computer. One way is to give a list, called an *adjacency list*, for each vertex listing all vertices adjacent to it. In the case of multiple edges, we list each adjacency as many times as there are edges that give the adjacency. In our pseudocode we implement the idea of an adjacency list with the array E that gives in position i a list of all locations in the array V of vertices adjacent in G to vertex $V[i]$.

In our pseudocode we also use an array "Edge" to list the edges of the set we called E' in algorithm Spantree, an array "Vertex" to list the positions in V of the vertices in the set S in the algorithm Spantree, an array "Vertexname" to keep track of the names of the vertices we add to the set S, and an array "Intree" to keep track of whether the vertex in position i of V is in S. Because we want our pseudocode to be easily translatable into a computer language, we avoid subscripts, and use x to stand for the place in the array V that holds the name of the vertex where we are to start the search, i.e. the vertex x_0.

```
BFSpantree(x,V,E)
// Assume that V is an array with v entries, the names of the vertices,
// and that x is the location in V of the name of the vertex with which we want
// to start the tree.
// Assume that E is an array with v entries, each a list of the positions
// in V of the names of vertices adjacent to the corresponding entry of V.
i = 0 ; k = 0 ; Intree[x] = 1; Vertex[0] = x; Vertexname[0] = V[x]
While i <= k
        i = i + 1
```

```
(4)         For each j in the list E[Vertex[i]]
(5)                 If Intree[j] ≠ 1
(6)                         k = k + 1
(7)                         Edge[k] = {V[Vertex[i]], V[j]}
(8)                         Intree[j] = 1
(9)                         Vertex[k] = j
(10)                        Vertexname[k] = V[j].
(11) Print "Connected component"
(12) return Vertexname[0 : k]
(13) print "Spanning tree edges of connected component"
(14) return Edge[1 : k]
```

Notice that the pseudocode allows us to deal with loops and multiple edges through the test whether vertex j is in the tree in Line 5. However the primary purpose of this line is to make sure that we do not examine edges that point from vertex i back to a vertex that is already in the tree.

This algorithm requires that we execute the "For" loop that starts in Line 4 once for each edge incident with vertex i. The "While" loop that starts in Line 2 is executed at most once for each vertex. Thus we execute the "For" loop at most twice for each edge, and carry out the other steps of the "While" loop at most once for each vertex, so that the time to carry out this algorithm is $O(V + E)$.

The algorithm carries out what is known as a "breadth first search"[5] of the graph centered at $V[x]$. The reason for the phrase "breadth first" is because each time we start to work on a new vertex, we examine all its edges (thus exploring the graph broadly at this point) before going on to another vertex. As a result, we first add all vertices at distance 1 from $V[x]$ to S, then all vertices at distance 2 and so on. When we choose a vertex $V[\text{Vertex}[k]]$ to put into the set S in Line 9, we are effectively labelling it as vertex k. We call k the *breadth first number* of the vertex $V[j]$ and denote it as $BFN(V[j])$[6]. The breadth first number of a vertex arises twice in the breadth first search algorithm. The breadth first search number of a vertex is assigned to that vertex when it is added to the tree, and (see Problem 7) is the number of vertices that have been previously added. But it then determines when a vertex of the tree is used to add other vertices to the tree: the vertices are taken in order of their breadth first number for the purpose of examining all incident edges to see which ones allow us to add new vertices, and thus new edges, to the tree.

This leads us to one more description of breadth first search. We create a breadth first search tree centered at x_0 in the following way. We put the vertex x_0 in the tree and give it breadth first number zero. Then we process the vertices in the tree in the order of their breadth first number as follows: We consider each edge leaving the vertex. If it is incident with a vertex z not in the tree, we put the edge into the edge set of the tree, we put z into the vertex set of the tree, and we assign z a breadth first number one more than that of the vertex most recently added to the tree. We continue in this way until all vertices in the tree have been processed.

We can use the idea of breadth first number to make our remark about the distances of vertices from x_0 more precise.

[5]This terminology is due to Robert Tarjan who introduced the idea in his PhD thesis.

[6]In words, we say that the breadth first number of a vertex is k if it is the kth vertex added to a breadth-first search tree, counting the initial vertex x as the zeroth vertex added to the tree

Lemma 6.7 *After a breadth first search of a graph G centered at $V[x]$, if $d(V[x], V[z]) > d(V[x], V[y])$, then BFN($V[z]$) >BFN($V[y]$).*

Proof: We will prove this in a way that mirrors our algorithm. We shall show by induction that for each nonnegative k, all vertices of distance k from x_0 are added to the spanning tree (that is, assigned a breadth first number and put into the set S) after all vertices of distance $k-1$ and before any vertices of distance $k+1$. When $k = 1$ this follows because S starts as the set $V[x]$ and all vertices adjacent to $V[x]$ are next added to the tree before any other vertices. Now assume that $n > 1$ and all vertices of distance n from $V[x]$ are added to the tree after all vertices of distance $n-1$ from $V[x]$ and before any vertices of distance $n+1$. Suppose some vertex of distance n added to the tree has breadth first number m. Then when i reaches m in Line 3 of our pseudocode we examine edges leaving vertex $V[\text{Vertex}[m]]$ in the "For loop." Since, by the inductive hypothesis, all vertices of distance $n-1$ or less from $V[x]$ are added to the tree before vertex $V[\text{Vertex}[m]]$, when we examine vertices $V[j]$ adjacent to vertex $V[\text{Vertex}[m]]$, we will have $\text{Intree}[j] = 1$ for these vertices. Since each vertex of distance n from $V[x]$ is adjacent to some vertex $V[z]$ of distance $n-1$ from $V[x]$, and $\text{BFN}[V[z]] < m$ (by the inductive hypothesis), any vertex of distance n from $V[x]$ and adjacent to vertex $V[\text{Vertex}[m]]$ will have $\text{Intree}[j] = 1$. Since any vertex adjacent to vertex $V[\text{Vertex}[m]]$ is of distance at most $n+1$ from $V[x]$, every vertex we add to the tree from vertex $V[\text{Vertex}[m]]$ will have distance $n+1$ from the tree. Thus every vertex added to the tree from a vertex of distance n from $V[x]$ will have distance $n+1$ from $V[x]$. Further, all vertices of distance $n+1$ are adjacent to some vertex of distance n from $V[x]$, so each vertex of distance $n+1$ is added to the tree from a vertex of distance n. Note that no vertices of distance $n+2$ from vertex $V[x]$ are added to the tree from vertices of distance n from vertex $V[x]$. Note also that all vertices of distance $n+1$ are added to the tree from vertices of distance n from vertex $V[x]$. Therefore all vertices with distance $n+1$ from $V[x]$ are added to the tree after all edges of distance n from $V[x]$ and before any edges of distance $n+2$ from $V[x]$. Therefore by the principle of mathematical induction, for every positive integer k, all vertices of distance k from $V[x]$ are added to the tree before any vertices of distance $k+1$ from vertex $V[x]$ and after all vertices of distance $k-1$ from vertex $V[x]$. Therefore since the breadth first number of a vertex is the number of the stage of the algorithm in which it was added to the tree, if $d(V[x], V[z]) > d(V[x], V[y])$, then BFN($V[z]$) >BFN($V[y]$). ■

Although we introduced breadth first search for the purpose of having an algorithm that quickly determines a spanning tree of a graph or a spanning tree of the connected component of a graph containing a given vertex, the algorithm does more for us.

Exercise 6.2-3 How does the distance from $V[x]$ to $V[y]$ in a breadth first search centered at $V[x]$ in a graph G relate to the distance from $V[x]$ to $V[y]$ in G?

In fact the unique path from $V[x]$ to $V[y]$ in a breadth first search spanning tree of a graph G is a shortest path in G, so the distance from $V[x]$ to another vertex in G is the same as their distance in a breadth first search spanning tree centered at $V[x]$. This makes it easy to compute the distance between a vertex $V[x]$ and all other vertices in a graph.

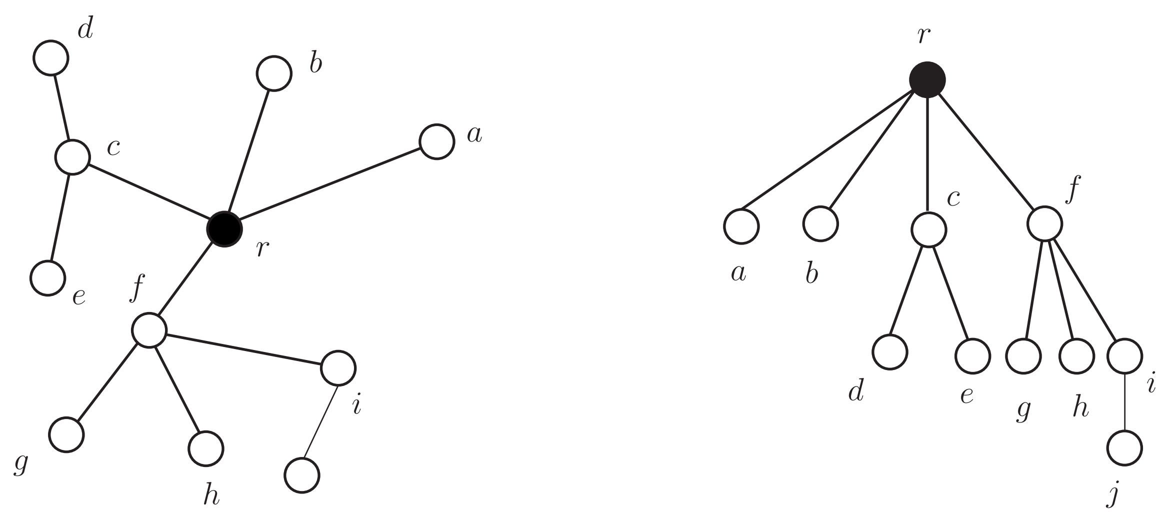
Theorem 6.8 *The unique path from $V[x]$ in a breadth first search spanning tree centered at the vertex $V[x]$ of a graph G to a vertex $V[y]$ is a shortest path from $V[x]$ to $V[y]$ in G.*

Proof: We prove the theorem by induction on the distance from $V[x]$ to $V[y]$. Fix a breadth first search tree of G centered at $V[x]$. If the distance is 0, then the single vertex $V[x]$ is a shortest path from $V[x]$ to $V[x]$ in G and the unique path in the tree. Assume that $k > 0$ and that when distance from $V[x]$ to $V[y]$ is less than k, the path from $V[x]$ to $V[y]$ in the tree is a shortest path from $V[x]$ to $V[y]$ in G. Now suppose that the distance from $V[x]$ to $V[y]$ is k. Suppose that a shortest path from $V[x]$ to $V[y]$ has $V[z]$ and $V[y]$ as its last two vertices. Suppose that the unique path from $V[x]$ to $V[y]$ in the tree has $V[z']$ and $V[y]$ as its last two vertices. Then $\mathrm{BFN}(V[z']) < \mathrm{BFN}(V[z])$, because otherwise we would have added $V[y]$ to the tree from vertex $V[z]$. Then by the contrapositive of Lemma 6.7, the distance from $V[x]$ to $V[z']$ is less than or equal to that from $V[x]$ to $V[z]$. But then by the inductive hypothesis, the distance from $V[x]$ to $V[z']$ is the length of the unique path in the tree, and by our previous comment is less than or equal to the distance from $V[x]$ to $V[z]$. However then the length of the unique path from $V[x]$ to $V[y]$ in the tree is no more than the distance from $V[x]$ to $V[y]$, so the two are equal. By the principle of mathematical induction, the distance from $V[x]$ to $V[y]$ is the length of the unique path in the tree for every vertex y of the graph. ■

Rooted Trees

A breadth first search spanning tree of a graph is not simply a tree, but a tree with a selected vertex, namely $V[x]$. It is one example of what we call a rooted tree. A *rooted tree* consists of a tree with a selected vertex, called a *root*, in the tree. Another kind of rooted tree you have likely seen is a binary search tree. It is fascinating how much additional structure is provided to a tree when we select a vertex and call it a root. In Figure 6.10 we show a tree with a chosen vertex and the result of redrawing the tree in a more standard way. The standard way computer scientists draw rooted trees is with the root at the top and all the edges sloping down, as you might expect to see with a family tree.

Figure 6.10: Two different views of the same rooted tree.



We adopt the language of family trees—ancestor, descendant, parent, and child—to describe rooted trees in general. In Figure 6.10, we say that vertex j is a child of vertex i, and a descendant of vertex r as well as a descendant of vertices f and i. We say vertex f is an ancestor of vertex i. Vertex r is the parent of vertices a, b, c, and f. Each of those four vertices is a child of vertex r. Vertex r is an ancestor of all the other vertices in the tree. In general, in a rooted tree with root r, a vertex x is an *ancestor* of a vertex y, and vertex y is a *descendant* of vertex x if x and y are different and x is on the unique path from the root to y. Vertex x is a *parent* of vertex y and y is a *child* of vertex x in a rooted tree if x is the unique vertex adjacent to y on the unique path from r to y. A vertex can have only one parent, but many ancestors. A vertex with no children is called a *leaf* vertex or an *external vertex*; other vertices are called *internal vertices*.

Exercise 6.2-4 Prove that a vertex in a rooted tree can have at most one parent. Does every vertex in a rooted tree have a parent?

In Exercise 6.2-4, suppose x is not the root. Then, because there is a unique path between a vertex x and the root of a rooted tree and there is a unique vertex on that path adjacent to x, each vertex other than the root has a unique parent. The root, however, has no parent.

Exercise 6.2-5 A binary tree is a special kind of rooted tree that has some additional structure that makes it tremendously useful as a data structure. In order to describe the idea of a binary tree it is useful to think of a tree with no vertices, which we call the null tree or empty tree. Then we can recursively describe a *binary tree* as

- an empty tree (a tree with no vertices), or
- a structure T consisting of a root vertex, a binary tree called the left subtree of the root and a binary tree called the right subtree of the root. If the left or right subtree is nonempty, its root node is joined by an edge to the root of T.

Then a single vertex is a binary tree with an empty right subtree and an empty left subtree. A rooted tree with two vertices can occur in two ways as a binary tree, either with a root and a left subtree consisting of one vertex or as a root and a right subtree consisting of one vertex. Draw all binary trees on four vertices in which the root node has an empty right child. Draw all binary trees on four vertices in which the root has a nonempty left child and a nonempty right child.

Exercise 6.2-6 A binary tree is a *full* binary tree if each vertex has either two nonempty children or two empty children (a vertex with two empty children is called a *leaf*.) Are there any full binary trees on an even number of vertices? Prove that what you say is correct.

For Exercise 6.2-5 we have five binary trees shown in Figure 6.11 for the first question. Then

Figure 6.11: The four-vertex binary trees whose root has an empty right child.

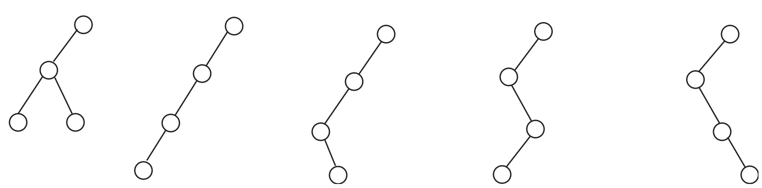
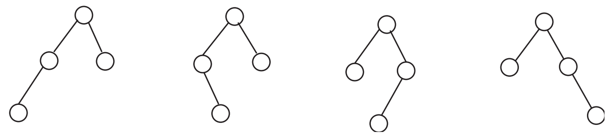


Figure 6.12: The four-vertex binary trees whose root has both a left and a right child.



in Figure 6.12 we have four more trees as the answer to the second question.

For Exercise 6.2-6, it is possible to have a full binary tree with zero vertices, so there is one such binary tree. But, if a full binary tree is not empty, it must have an odd number of vertices. We can prove this inductively. A full binary tree with 1 vertex has an odd number of vertices. Now suppose inductively that $n > 1$ and any full binary tree with fewer than n vertices has an odd number of vertices. For a full binary tree with $n > 1$ vertices, the root must have two nonempty children. Thus removing the root gives us two binary trees, rooted at the children of the original root, each with fewer than n vertices. By the definition of full, each of the subtrees rooted in the two children must be full binary tree. The number of vertices of the original tree is one more than the total number of vertices of these two trees. This is a sum of three odd numbers, so it must be odd. Thus, by the principle of mathematical induction, if a full binary tree is not empty, it must have odd number of vertices.

The definition we gave of a binary tree was an inductive one, because the inductive definition makes it easy for us to prove things about binary trees. We remove the root, apply the inductive hypothesis to the binary tree or trees that result, and then use that information to prove our result for the original tree. We could have defined a binary tree as a special kind of rooted tree, such that

- each vertex has at most two children,
- each child is specified to be a left or right child, and
- a vertex has at most one of each kind of child.

While it works, this definition is less convenient than the inductive definition.

There is a similar inductive definition of a *rooted tree*. Since we have already defined rooted trees, we will call the object we are defining an r-tree. The recursive definition states that an r-tree is either a single vertex, called a root, or a graph consisting of a vertex called a root and a set of disjoint r-trees, each of which has its root attached by an edge to the original root. We can then prove as a theorem that a graph is an r-tree if and only if it is a rooted tree. Sometimes inductive proofs for rooted trees are easier if we use the method of removing the root and applying the inductive hypothesis to the rooted trees that result, as we did for binary trees in our solution of Exercise 6.2-6.

Important Concepts, Formulas, and Theorems

1. *Spanning Tree.* A tree whose edge set is a subset of the edge set of the graph G is called a *spanning tree* of G if the tree has exactly the same vertex set as G.

2. *Breadth First Search.* We create a *breadth first search* tree centered at x_0 in the following way. We put the vertex x_0 in the tree and give it breadth first number zero. Then we process the vertices in the tree in the order of their breadth first number as follows: We consider each edge leaving the vertex. If it is incident with a vertex z not in the tree, we put the edge into the edge set of the tree, we put z into the vertex set of the tree, and we assign z a breadth first number one more than that of the vertex most recently added to the tree. We continue in this way until all vertices in the tree have been processed.

3. *Breadth first number.* The *breadth first number* of a vertex in a breadth first search tree is the number of vertices that were already in the tree when the vertex was added to the vertex set of the tree.

4. *Breadth first search and distances.* The distance from a vertex y to a vertex x may be computed by doing a breadth first search centered at x and then computing the distance from y to x in the breadth first search tree. In particular, the path from x to y in a breadth first search tree of G centered at x is a shortest path from x to y in G.

5. *Rooted tree.* A *rooted tree* consists of a tree with a selected vertex, called a *root*, in the tree.

6. *Ancestor, Descendant.* In a rooted tree with root r, a vertex x is an *ancestor* of a vertex y, and vertex y is a *descendant* of vertex x if x and y are different and x is on the unique path from the root to y.

7. *Parent, Child.* In a rooted tree with root r, vertex x is a *parent* of vertex y and y is a *child* of vertex x in if x is the unique vertex adjacent to y on the unique path from r to y.

8. *Leaf (External) Vertex.* A vertex with no children in a rooted tree is called a *leaf* vertex or an *external vertex*.

9. *Internal Vertex.* A vertex of a rooted tree that is not a leaf vertex is called an *internal* vertex.

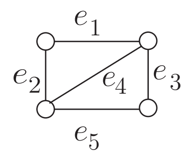
10. *Binary Tree.* We recursively describe a *binary tree* as

    - an empty tree (a tree with no vertices), or
    - a structure T consisting of a root vertex, a binary tree called the left subtree of the root and a binary tree called the right subtree of the root. If the left or right subtree is nonempty, its root node is joined by an edge to the root of T.

11. *Full Binary Tree.* A binary tree is a *full* binary tree if each vertex has either two nonempty children or two empty children.

12. *Recursive Definition of a Rooted Tree.* The recursive definition of a rooted tree states that it is either a single vertex, called a root, or a graph consisting of a vertex called a root and a set of disjoint rooted trees, each of which has its root attached by an edge to the original root.

Figure 6.13: A graph.



Problems

1. Find all spanning trees (list their edge sets) of the graph in Figure 6.13.

2. Show that a finite graph is connected if and only if it has a spanning tree.

3. Draw all rooted trees on 5 vertices. The order and the place in which you write the vertices down on the page is unimportant. If you would like to label the vertices (as we did in the graph in Figure 6.10), that is fine, but don't give two different ways of labelling or drawing the same tree.

4. Draw all rooted trees on 6 vertices with four leaf vertices. If you would like to label the vertices (as we did in the graph in Figure 6.10), that is fine, but don't give two different ways of labelling or drawing the same tree.

5. Find a tree with more than one vertex that has the property that all the rooted trees you get by picking different vertices as roots are different as rooted trees. (Two rooted trees are the same (isomorphic), if they each have one vertex or if you can label them so that they have the same (labelled) root and the same (labelled) subtrees.)

6. Create a breadth first search tree centered at vertex 12 for the graph in Figure 6.8 and use it to compute the distance of each vertex from vertex 12. Give the breadth first number for each vertex.

7. It may seem clear to some people that the breadth first number of a vertex is the number of vertices previously added to the tree. However the breadth first number was not actually defined in this way. Give a proof that the breadth first number of a vertex is the number of vertices previously added to the tree.

8. A *(left, right) child* of a vertex in a binary tree is the root of a (left, right) subtree of that vertex. A binary tree is a *full* binary tree if each vertex has either two nonempty children or two empty children (a vertex with two empty children is called a *leaf*.) Draw all full binary trees on seven vertices.

9. The *depth* of a node in a rooted tree is defined to be the number of edges on the (unique) path to the root. A binary tree is *complete* if it is full (see Problem 8) and all its leaves have the same depth. How many vertices does a complete binary tree of depth 1 have? Depth 2? Depth d? (Proof required for depth d.)

10. The *height* of a rooted or binary tree with one vertex is 0; otherwise it is 1 plus the maximum of the heights of its subtrees. Based on Exercise 6.2-9, what is the minimum height of *any* binary tree on n vertices? (Please prove this.)

11. A binary tree is complete if it is full and all its leaves have the same depth (see Exercise 6.2-8 and Exercise 6.2-9). A vertex that is not a leaf vertex is called an *internal* vertex. What is the relationship between the number I of internal vertices and the number L of leaf vertices in a complete binary tree. A full binary tree? (Proof please.)

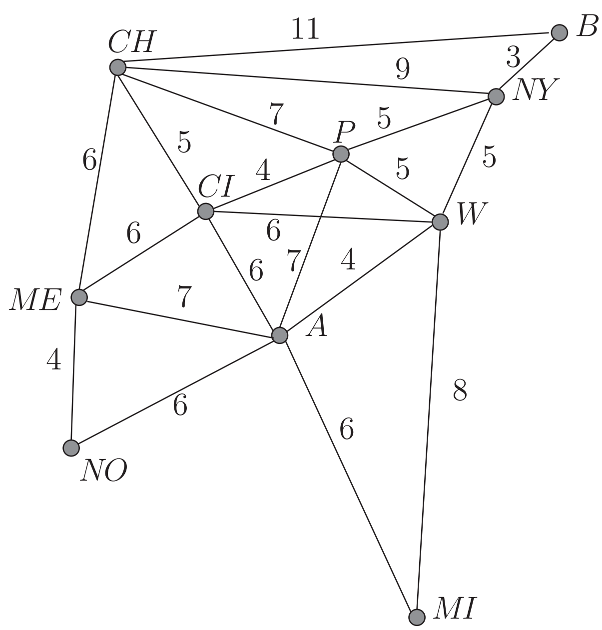
12. The *internal path length* of a binary tree is the sum, taken over all internal (see Exercise 6.2-11) vertices of the tree, of the depth of the vertex. The *external path length* of a binary tree is the sum, taken over all leaf vertices of the tree, of the depth of the vertex. Show that in a full binary tree with n internal vertices, internal path length i and external path length e, we have $e = i + 2n$.

13. Prove that a graph is an r-tree, as defined at the end of the section if and only if it is a rooted tree.

14. Use the inductive definition of a rooted tree (r-tree) given at the end of the section to prove once again that a rooted tree with n vertices has $n - 1$ edges if $n \geq 1$.

15. In Figure 6.14 we have added numbers to the edges of the graph of Figure 6.1 to give what is usually called a *weighted graph*—the name for a graph with numbers, often called *weights* associated with its edges. We use $w(\epsilon)$ to stand for the weight of the edge ϵ. These numbers represent the lease fees in thousands of dollars for the communication lines the edges represent. Since the company is choosing a spanning tree from the graph to save money, it is natural that it would want to choose the spanning tree with minimum total cost. To be precise, a *minimum spanning tree* in a weighted graph is a spanning tree of the graph such that the sum of the weights on the edges of the spanning tree is a minimum among all spanning trees of the graph.

Figure 6.14: A stylized map of some eastern US cities.



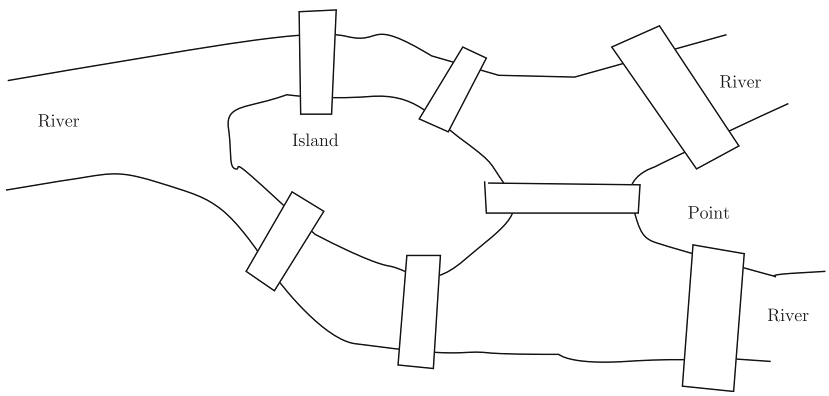
Give an algorithm to select a spanning tree of minimum total weight from a weighted graph and apply it to find a minimum spanning tree of the weighted graph in Figure 6.14. Show that your algorithm works and analyze how much time it takes.

6.3 Eulerian and Hamiltonian Paths and Tours

Eulerian Tours and Trails

Exercise 6.3-1 In an article generally acknowledged to be one of the origins of the graph theory [7] Leonhard Euler (pronounced Oiler) described a geographic problem that he offered as an elementary example of what he called "the geometry of position." The problem, known as the "Königsberg Bridge Problem," concerns the town of Königsberg in Prussia (now Kaliningrad in Russia), which is shown in a schematic map (circa 1700) in Figure 6.15. Euler tells us that the citizens amused themselves

Figure 6.15: A schematic map of Königsberg

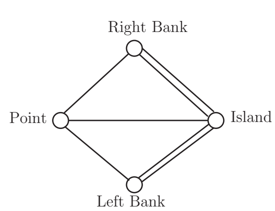


by trying to find a walk through town that crossed each of the seven bridges once and only once (and, hopefully, ended where it started). Is such a walk possible?

In Exercise 6.3-1, such a walk will enter a land mass on a bridge and leave it on a different bridge, so except for the starting and ending point, the walk requires two new bridges each time it enters and leaves a land mass. Thus each of these land masses must be at the end of an even number of bridges. However, as we see from Figure 6.15 each land mass is at the end of an odd number of bridges. Therefore no such walk is possible.

We can represent the map in Exercise 6.3-1 more compactly with the graph in Figure 6.16. In graph theoretic terminology Euler's question asks whether there is a path, starting and ending

Figure 6.16: A graph to replace the schematic map of Königsberg



[7] Reprinted in *Graph Theory 1736-1936* by Biggs, Lloyd and Wilson (Clarendon, 1976)

at the same vertex, that uses each edge exactly once.

Exercise 6.3-2 Determine whether the graph in Figure 6.1 has a closed path that includes each edge of the graph exactly once, and find one if it does.

Exercise 6.3-3 Find the strongest condition you can that has to be satisfied by a graph that has a path, starting and ending at the same place, that includes each vertex at least once and each edge once and only once. Such a path is known as an *Eulerian Tour* or *Eulerian Circuit*.

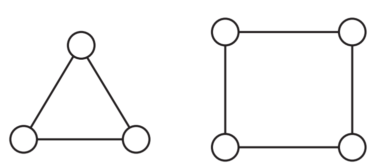
Exercise 6.3-4 Find the strongest condition you can that has to be satisfied by a graph that has a path, starting and ending at different places, that includes each vertex at least once and each edge once and only once. Such a path is known as an *Eulerian Trail*

Exercise 6.3-5 Determine whether the graph in Figure 6.1 has an Eulerain Trail and find one if it does.

The graph in Figure 6.1 cannot have a closed path that includes each edge exactly once because if the initial vertex of the path were P, then the number of edges incident with P would have to be one at the beginning of the path, plus two for each time P appears before the end of the path, plus one more for the time P would appear at the end of the path, so the degree of P would have to be even. But if P were not the initial vertex of a closed path including all the edges, each time we entered P on one edge, we would have to leave it on a second edge, so the number of edges incident with P would have to be even. Thus in Exercise 6.3-2 there is no closed path that includes each edge exactly once.

Notice that, just as we argued for a walk through Königsberg, in any graph with an Eulerian Circuit, each vertex except for the starting-finishing one will be paired with two new edges (those preceding and following it on the path) each time it appears on the path. Therefore each of these vertices is incident with an even number of edges. Further, the starting vertex is incident with one edge at the beginning of the path and is incident with a different edge at the end of the path. Each other time it occurs, it will be paired with two edges. Thus this vertex is incident with an even number of edges as well. Therefore a natural condition a graph must satisfy if it has an Eulerian Tour is that each vertex has even degree. But Exercise 6.3-3 asked us for the strongest condition we could find that a graph with an Eulerian Tour would satisfy. How do we know whether this is as strong a condition as we could devise? In fact it isn't, the graph in Figure 6.17 clearly has no Eulerian Tour because it is disconnected, but every vertex has even degree.

Figure 6.17: This graph has no Eulerian Tour, even though each vertex has even degree.



The point that Figure 6.17 makes is that in order to have an Eulerian Tour, a graph must be connected as well as having only vertices of even degree. Thus perhaps the strongest condition we can find for having an Eulerian Tour is that the graph is connected and every vertex has even degree. Again, the question comes up "How do we show this condition is as strong as possible, if indeed it is?" We showed a condition was not as strong as possible by giving an example of a graph that satisfied the condition but did not have an Eulerian Tour. What if we could show that no such example is possible, i.e. we could prove that a graph which is connected and in which every vertex has even degree does have an Eulerian Tour? Then we would have shown our condition is as strong as possible.

Theorem 6.9 *A graph has an Eulerian Tour if and only if it is connected and each vertex has even degree.*

Proof: A graph must be connected to have an Eulerian tour, because there must be a path that includes each vertex, so each two vertices are joined by a path. Similarly, as explained earlier, each vertex must have even degree in order for a graph to have an Eulerian Tour. Therefore we need only show that if a graph is connected and each vertex has even degree, then it has an Eulerain Tour. We do so with a recursive construction. If G has one vertex and no edges, we have an Eulerian tour consisting of one vertex and no edges. So suppose G is connected, has at least one edge, and each vertex of G has even degree. Now, given distinct vertices x_0, x_1, …, x_i and edges ϵ_1, ϵ_2, …, ϵ_i such that $x_0\epsilon_1x_1\dots\epsilon_ix_i$ is a path, choose an edge ϵ_{i+1} from x_i to a vertex x_{j+1}. If x_{j+1} is x_0, stop. Eventually this process must stop because G is finite, and (since each vertex in G has even degree) when we enter a vertex other than x_0, there will be an edge on which we can leave it. This gives us a closed path C. Delete the edges of this closed path from the edge set of G. This gives us a graph G' in which each vertex has even degree, because we have removed two edges incident with each vertex of the closed path (or else we have removed a loop). However, G' need not be connected. Each connected component of G' is a connected graph in which each vertex has even degree. Further, each connected component of G' contains at least one element x_i. (Suppose a connected component C contained no x_i. Since G is connected, for each i, there is a path in G from each vertex in C to each vertex x_i. Choose the shortest such path, and suppose it connects a vertex y in C to x_j. Then no edge in the path can be in the closed path, or else we would have a shorter path from y to a different vertex x_i. Therefore removing the edges of the closed path leaves y connected to x_j in C, so that C contains an x_i after all, a contradiction.) We may assume inductively that each connected component has fewer edges than G, so each connected component has an Eulerian Tour. Now we may begin to recursively construct an Eulerian Tour of G by starting at x_j, and taking an Eulerian Tour of the connected component containing x_j. Then given a sequence x_j, x_1, …, x_k such that the Eulerian tour we have constructed so far includes the vertices x_j through x_k, the vertices and edges of the connected components of G' containing the vertices x_k through x_k, the edges ϵ_{j+1} through ϵ_k, we add the edge e_{k+1} and the vertex x_{k+1} to our tour, and if the vertices and edges of the connected component of G' containing x_{k+1} are not already in our tour, we add an Eulerian Tour of the connected component of G' containing x_{k+1} to our tour. When we add the last edge and vertex of our closed path to the path we have been constructing, every vertex and edge of the graph will have to be in the path we have constructed, because every vertex is in some connected component of G', and every edge is either an edge of the first closed path or an edge of some connected component of G'. Therefore if G is connected and each vertex of G has even degree, then G has an Eulerian Tour. ■

A graph with an Eulerian Tour is called an *Eulerian Graph*.

In Exercise 6.3-4, each vertex other than the initial and final vertices of the walk must have even degree by the same reasoning we used for Eulerian tours. But the initial vertex must have odd degree, because the first time we encounter it in our Eulerian Trail it is incident with one edge in the path, but each succeeding time it is incident with two edges in the path. Similarly the final vertex must have odd degree. This makes it natural to guess the following theorem.

Theorem 6.10 *A graph G has an Eulerian Trail if and only if G is connected and all but two of the vertices of G have even degree.*

Proof: We have already shown that if G has an Eulerian Trail, then all but two vertices of G have even degree and these two vertices have odd degree.

Now suppose that G is a connected graph in which all but two vertices have even degree. Suppose the two vertices of odd degree are x and y. Add an edge ϵ joining x and y to the edge set of G to get G'. Then G' has an Eulerian Tour by Theorem 6.9. One of the edges of the tour is the added edge. We may traverse the tour starting with any vertex and any edge following that vertex in the tour, so we may begin the tour with either $x\epsilon y$ or $y\epsilon x$. By removing the first vertex and ϵ from the tour, we get an Eulerian Trail. ■

By Theorem 6.10, there is no Eulerian Trail in Exercise 6.3-5.

Notice that our proof of Theorem 6.9 gives us a recursive algorithm for constructing a Tour. Namely, we find a closed walk W starting and ending at a vertex we choose, identify the connected components of the graph $G - W$ that results from removing the closed walk, and then follow our closed walk, pausing each time we enter a new connected component of $G - W$ to recursively construct an Eulerian Tour of the component and traverse it before returning to following our closed walk. It is possible that the closed walk we remove has only one edge (or in the case of a simple graph, some very small number of edges), and the number of steps needed for a breadth first search is $\Theta(e')$, where e' the number of edges in the graph we are searching. Thus our construction could take $\Theta(e)$ steps, each of which involves examining $\Theta(e)$ edges, and therefore our algorithm takes $O(e^2)$ time. (We get a big Oh bound and not a big Theta bound because it is also possible that the closed walk we find the first time is an Eulerian tour.)

It is an interesting observation on the progress of mathematical reasoning that Euler made a big deal in his paper of explaining why it is necessary for each land mass to have an even number of bridges, but seemed to consider the process of constructing the path rather self-evident, as if it was hardly worth comment. For us, on the other hand, proving that the construction is possible if each land mass has an even number of bridges (that is, showing that the condition that each land mass has an even number of bridges is a sufficient condition for the existence of an Eulerian tour) was a much more significant effort than proving that having an Eulerian tour requires that each land mass has an even number of bridges. The standards of what is required in order to back up a mathematical claim have changed over the years.

Hamiltonian Paths and Cycles

A natural question to ask in light of our work on Eulerian tours is whether we can state necessary and sufficient conditions for a graph to have a closed path that includes each vertex exactly once (except for the beginning and end). An answer to this question would have the potential to be quite useful. For example, a salesperson might have to plan a trip through a number of cities which are connected by a network of airline routes. Planning the trip so the salesperson would travel through a city only when stopping there for a sales call would minimize the number of flights the needed. This question came up in a game, called "around the world," designed by William Rowan Hamilton. In this game the vertices of the graph were the vertices of a dodecahedron (a twelve sided solid in which each side is a pentagon), and the edges were the edges of the solid. The object was to design a trip that started at one vertex and visited each vertex once and then returned to the starting vertex along an edge. Hamilton suggested that players could take turns, one choosing the first five cities on a tour, and the other trying to complete the tour. It is because of this game that a cycle that includes each vertex of the graph exactly once (thinking of the first and last vertex of the cycle as the same) is called a *Hamiltonian Cycle*. A graph is called Hamiltonian if it has a Hamiltonian cycle.. A *Hamiltonian Path* is a simple path that includes each vertex of the graph exactly once. It turns out that nobody yet knows (and as we shall explain briefly at the end of the section, it may be reasonable to expect that nobody will find) uesful necessary and sufficient conditions for a graph to have a Hamiltonian Cycle or a Hamiltonian Path that are significantly easier to verify than trying all permutations of the vertices to see if taking the vertices in the order of that permutation to see if that order defines a Hamiltonian Cycle or Path. For this reason this branch of graph theory has evolved into theorems that give sufficient conditions for a graph to have a Hamiltonian Cycle or Path; that is theorems that say all graphs of a certain type have Hamiltonian Cycles or Paths, but do not characterize all graphs that have Hamiltonian Cycles of Paths.

Exercise 6.3-6 Describe all values of n such that a complete graph on n vertices has a Hamiltonian Path. Describe all values of n such that a complete graph on n vertices has a Hamiltonian Cycle.

Exercise 6.3-7 Determine whether the graph of Figure 6.1 has a Hamiltonian Cycle or Path, and determine one if it does.

Exercise 6.3-8 Try to find an interesting condition involving the degrees of the vertices of a simple graph that guarantees that the graph will have a Hamiltonian cycle. Does your condition apply to graphs that are not simple? (There is more than one reasonable answer to this exercise.)

In Exercise 6.3-6, the path consisting of one vertex and no edges is a Hamiltonian path but not a Hamiltonian cycle in the complete graph on one vertex. (Recall that a path consisting of one vertex and no edges is not a cycle.) Similarly, the path with one edge in the complete graph K_2 is a Hamiltonian path but not a Hamiltonian cycle, and since K_2 has only one edge, there is no Hamiltonian cycle in the K_2. In the complete graph K_n, any permutation of the vertices is a list of the vertices of a Hamiltonian path, and if $n > 3$, such a Hamiltonian Path from x_1 to x_n, followed by the edge from x_n to x_1 and the vertex x_1 is a Hamiltonian Cycle. Thus each complete graph has a Hamiltonian Path, and each complete graph with more than three vertices has a Hamiltonian Cycle.

In Exercise 6.3-7, the path with vertices NO, A, MI, W, P, NY, B, CH, CL, and ME is a Hamiltonian Path, and adding the edge from ME to NO gives a Hamiltonian Cycle.

Based on our observation that the complete graph on n vertices has a Hamiltonian Cycle if $n > 2$, we might let our condition be that the degree of each vertex is one less than the number of vertices, but this would be uninteresting since it would simply restate what we already know for complete graphs. The reason why we could say that K_n has a Hamiltonian Cycle when $n > 3$ was that when we entered a vertex, there was always an edge left on which we could leave the vertex. However the condition that each vertex has degree $n-1$ is stronger than we needed, because until we were at the second-last vertex of the cycle, we had more choices than we needed for edges on which to leave the vertex. On the other hand, it might seem that even if n were rather large, the condition that each vertex should have degree $n-2$ would not be sufficient to guarantee a Hamiltonian cycle, because when we got to the second last vertex on the cycle, all of the $n-2$ vertices it is adjacent to might already be on the cycle and different from the first vertex, so we would not have an edge on which we could leave that vertex. However there is the possibility that when we had some choices earlier, we might have made a different choice and thus included this vertex earlier on the cycle, giving us a different set of choices at the second last vertex. In fact, if $n > 3$ and each vertex has degree at least $n-2$, then we could choose vertices for a path more or less as we did for the complete graph until we arrived at vertex $n-1$ on the path. Then we could complete a Hamiltonian path unless x_{n-1} was adjacent only to the first $n-2$ vertices on the path. In this last case, the first $n-1$ vertices would form a cycle, because x_{n-1} would be adjacent to x_1. Suppose y was the vertex not yet on the path. Since y has degree $n-2$ and y is not adjacent to x_{n-1}, y would have to be adjacent to the first $n-2$ vertices on the path. Then since $n > 3$, we could take the path $x_1 y x_2 \ldots x_{n-1} x_1$ and we would have a Hamiltonian cycle. Of course unless n were four, we could also insert y between x_2 and x_3 (or any x_{i-1} and x_i such that $i < n-1$, so we would still have a great deal of flexibility. To push this kind of reasoning further, we will introduce a new technique that often appears in graph theory. We will point out our use of the technique after the proof.

Theorem 6.11 (Dirac) *If every vertex of a v-vertex simple graph G with at least three vertices has degree at least $v/2$, then G has a Hamiltonian cycle.*

Proof: Suppose, for the sake of contradiction that there is a graph G_1 with no Hamiltonian Cycle in which each vertex has degree at least $v/2$. If we add edges joining existing vertices to G_1, each vertex will still have degree at least $v/2$. If add all possible edges to G_1 we will get a complete graph, and it will have a Hamiltonian cycle. Thus if we continue adding edges to G_1, we will at some point reach a graph that does have a Hamiltonian cycle. Instead, we add edges to G_1 until we reach a graph G_2 that has no Hamiltonian cycle but has the property that if we add any edge to G_2, we get a Hamiltonian cycle. We say G_2 is *maximal* with respect to not having a Hamiltonian cycle. Suppose x and y are not adjacent in G_2. Then adding an edge between x and y to G_2 gives a graph with a Hamiltonian cycle, and x and y must be connected by the added edge in this Hamiltonian cycle. (Otherwise G_2 would have a Hamiltonian cycle.) Thus G_2 has a Hamiltonian path $x_1 x_2 \ldots x_v$ that starts at $x = x_1$ and ends at $y = x_v$. Further x and y are not adjacent.

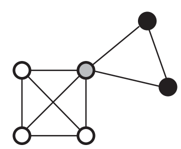
Before we stated our theorem we considered a case where we had a cycle on $f-1$ vertices and were going to put an extra vertex into it between two adjacent vertices. Now we have a path on f vertices from $x = x_1$ to $y = x_f$, and we want to convert it to a cycle. If we had that y is adjacent to some vertex x_i on the path while x is adjacent to x_{i+1}, then we could construct the Hamiltonian cycle $x_1 x_{i+1} x_{i+2} \ldots x_f x_i x_{i-1} \ldots x_2 x_1$. But we are assuming our graph does not have a Hamiltonian cycle. Thus for each x_i that x is adjacent to on the path $x_1 x_2 \ldots x_v$, y is not adjacent to x_{i-1}. Since all vertices are on the path, x is adjacent to at least $v/2$ vertices among x_2 through x_v. Thus y is not adjacent to at least $v/2$ vertices among x_1 through x_{v-1}. But there are only $v-1$ vertices, namely x_1 through x_{v-1}, vertices y could be adjacent to, since it is not adjacent to itself. Thus y is adjacent at most $v-1-v/2 = v/2-1$ vertices, a contradiction. Therefore if each vertex of a simple graph has degree at least $v/2$, the graph has a Hamiltonian Cycle. ■ The new tachnique was that of assuming we had a maximal graph (G_2) that did not have our desired property and then using this maximal graph in a proof by contradiction.

Exercise 6.3-9 Suppose $v = 2k$ and consider a graph G consisting of two complete graphs, one with k vertices, $x_1, \ldots x_k$ and one with $k+1$ vertices, $x_k, \ldots x_{2k}$. Notice that we get a graph with exactly $2k$ vertices, because the two complete graphs have one vertex in common. How do the degrees of the vertices relate to v? Does the graph you get have a Hamiltonian cycle? What does this say about whether we can reduce the lower bound on the degree in Theorem 6.11?

Exercise 6.3-10 In the previous exercise, is there a similar example in the case $v = 2k+1$?

In Exercise 6.3-9, the vertices that lie in the complete graph with k vertices, with the exception of x_k, have degree $k-1$. Since $v/2 = k$, this graph does not satisfy the hypothesis of Dirac's theorem which assumes that every vertex of the graph has degree at least $v/2$. We show the case in which $k = 3$ in Figure 6.18.

Figure 6.18: The vertices of K_4 are white or grey; those of K_3 are black or grey.



You can see that the graph in Figure 6.18 has no Hamiltonian cycle as follows. If an attempt at a Hamiltonian cycle begins at a white vertex, after crossing the grey vertex to include the black ones, it can never return to a white vertex without using the grey one a second time. The situation is similar if we tried to begin a Hamiltonian cycle at a black vertex. If we try to begin a Hamiltonian cycle at the grey vertex, we would next have to include all white vertices or all black vertices in our cycle and would then be stymied because we would have to take our path through the grey vertex a second time to change colors between white and black. As long as $k \geq 2$, the same argument shows that our graph has no Hamiltonian cycle. Thus the lower bound of $v/2$ in Dirac's theorem is tight; that is, we have a way to construct a graph with minimum degree $v/2-1$ (when v is even) for which there is no Hamiltonian cycle. If $v = 2k+1$ we might consider two complete graphs of size $k+1$, joined at a single vertex. Each vertex other than the one at which they are joined would have degree k, and we would have $k < k+1/2 = v/2$, so again the minimum degree would be less than $v/2$. The same kind of argument that we used with the graph in Figure 6.18 would show that as long as $k \geq 1$, we have no Hamiltonian cycle.

If you analyze our proof of Dirac's theorem, you will see that we really used only a consequence of the condition that all vertices have degree at least $v/2$, namely that for any two vertices, the sum of their degrees is at least n.

Theorem 6.12 (Ore) *If G is a v-vertex simple graph with $n \geq 3$ such that for each two nonadjacent vertices x and y the sum of the degrees of x and y is at least v, then G has a Hamiltonian cycle.*

Proof: See Problem 13. ■

NP-Complete Problems

As we began the study of Hamiltonian Cycles, we mentioned that the problem of determining whether a graph has a Hamiltonian Cycle seems significantly more difficult than the problem of determining whether a graph has a Eulerian Tour. On the surface these two problems have significant similarities.

- Both problems whether a graph has a particular property. (Does this graph have a Hamiltonian/Eulerian closed path?) The answer is simply yes or no.
- For both problems, there is additional information we can provide that makes it relatively easy to check a yes answer if there is one. (The additional information is a closed path. We simply check whether the closed path includes each edge or each vertex exactly once.)

But there is a striking difference between the two problems as well. It is reasonably easy to find an Eulerian path in a graph that has one (we saw that the time to use the algorithm implicit in the proof of Theorem 6.9 is $O(e^2)$ where e is the number of edges of the graph. However, nobody knows how to actually find a permutation of the vertices that is a Hamiltonian path without checking essentially all permutations of the vertices.[8] This puts us in an interesting position. Although if someone gets lucky and guesses a permutation that is a Hamiltonian path, we can quickly verify the person's claim to have a Hamiltonian path, but in a graph of reasonably large size we have no practical method for finding a Hamiltonian path.

This difference is the essential difference between the class **P** of problems said to be solvable in polynomial time and the class **NP** of problems said to be solvable in nondeterministic polynomial time. We are not going to describe these problem classes in their full generality. A course in formal languages or perhaps algorithms is a more appropriate place for such a discussion. However in order to give a sense of the difference between these kinds of problems, we will talk about them in the context of graph theory. A question about whether a graph has a certain property is called a *graph decision problem*. Two examples are the question of whether a graph has an Eulerian tour and the question of whether a graph has a Hamiltonian cycle.

A graph decision problem has a yes/no answer. A **P**-*algorithm* or polynomial time algorithm for a property takes a graph as input and in time $O(n^k)$, where k is a positive integer independent of the input graph and n is a measure of the amount of information needed to specify the input graph, it outputs the answer "yes" if and only if the graph does have the property. We say the algorithm *accepts* the graph if it answers yes. (Notice we don't specify what the algorithm does if the graph does not have the property, except that it doesn't output yes.) We say a property of graphs is *in the class* **P** if there is a **P**-algorithm that accepts exactly the graphs with the property.

An **NP**-algorithm (non-deterministic polynomial time) for a property takes a graph and $O(n^j)$ additional information, and in time $O(n^k)$, where k and j are positive integers independent of

[8]We say essentially because one can eliminate some permutations immediately; for example if there is no edge between the first two elements of the permutation, then not only can we ignore the rest of this permutation, but we may ignore any other permutation that starts in this way. However nobody has managed to find a sub-exponential time algorithm for solving the Hamiltonian cycle problem.

the the input graph and n is a measure of the amount of information needed to specify the input graph, outputs the answer yes if and only if it can use the additional information to determine that the graph has the property. For example for the property of being Hamiltonian, the algorithm might input a graph and a permutation of the vertex set of the graph. The algorithm would then check the permutation to see if it lists the vertices in the order of a Hamiltonian cycle and output "yes" if it does. We say the algorithm *accepts* a graph if there is additional information it can use with the graph as an input to output "yes." We call such an algorithm nondeterministic, because whether or not it accepts a graph is determined not merely by the graph but by the additional information as well. In particular, the algorithm might or might not accept every graph with the given property. We say a property is *in the class* **NP** if there is an **NP**-algorithm that accepts exactly the graphs with the property. Since graph decision problems ask us to decide whether or not a graph has a given problem, we adopt the notation **P** and **NP** to describe problems as well. We say a decision problem is in **P** or **NP** if the graph property it asks us to decide is in **P** or **NP** respectively.

When we say that a nondeterministic algorithm uses the additional information, we are thinking of "use" in a very loose way. In particular, for a graph decision problem in **P**, the algorithm could simply ignore the additional information and use the polynomial time algorithm to determine whether the answer should be yes. Thus every graph property in **P** is also in **NP** as well. The question as to whether **P** and **NP** are the same class of problems has vexed computer scientists since it was introduced in 1968.

Some problems in **NP**, like the Hamiltonian path problem have an exciting feature: any instance[9] of any problem in **NP** can be translated in $O(n^k)$ steps, where n and k are as before, into $O(n^j)$ instances of the Hamilton path problem, where j is independent of n and k. In particular, the answer to the original problem is yes if and only if the answer to one of the Hamiltonian path problems is yes. The translation preserves whether or not the graph in the original instance of the problem is accepted. We say that the Hamiltonian Path problem is **NP**-complete. More generally, a problem in **NP** is called **NP**-complete if, for each other problem in **NP**, we can devise an algorithm for the second problem that has $O(n^k)$ steps (where n is a measure of the size of the input graph, and k is independent of n), including counting as one step solving an instance of the first problem, and accepts exactly the instances of the second problem that have a yes answer. The question of whether a graph has a clique (a subgraph that is a complete graph) of size j is another problem in **NP** that is **NP**-complete. In particular, if one **NP** complete problem has a polynomial time algorithm, every problem in NP is in **P**. Thus we can determine in polynomial time whether an arbitrary graph has a Hamiltonian path if and only if we can determine in polynomial time whether an arbitrary graph has a clique of (an arbitrary) size j. Literally hundreds of interesting problems are NP-complete. Thus a polynomial time solution to any one of them would provide a polynomial time solution to all of them. For this reason, many computer scientists consider a demonstration that a problem is NP-complete to be a demonstration that it is unlikely to be solved by a polynomial time algorithm.

This brief discussion of NP-completeness is intended to give the reader a sense of the nature and importance of the subject. We restricted ourselves to graph problems for two reasons. First, we expect the reader to have a sense of what a graph problem is. Second, no treatment of graph theory is complete without at least some explanation of how some problems seem to be much more intractable than others. However, there are **NP**-complete problems throughout mathematics and

[9]An instance of a problem is a case of the problem in which all parameters are specified; for example a particular instance of the Hamiltonian Cycle problem is a case of the problem for a particular graph.

computer science. Providing a real understanding of the subject would require much more time than is available in an introductory course in discrete mathematics.

Important Concepts, Formulas, and Theorems

1. A graph that has a path, starting and ending at the same place, that includes each vertex at least once and each edge once and only once is called an *Eulerian Graph.* Such a path is known as an *Eulerian Tour* or *Eulerian Circuit.*

2. A graph has an Eulerian Tour if and only if it is connected and each vertex has even degree.

3. A path that includes each vertex of the graph at least once and each edge of the graph exactly once, but has different first and last endpoints, is known as an *Eulerian Trail*

4. A graph G has an Eulerian Trail if and only if G is connected and all but two of the vertices of G have even degree.

5. A cycle that includes each vertex of a graph exactly once (thinking of the first and last vertex of the cycle as the same) is called a *Hamiltonian Cycle.* A graph is called Hamiltonian if it has a Hamiltonian cycle.

6. A *Hamiltonian Path* is a simple path that includes each vertex of the graph exactly once.

7. (Dirac's Theorem) If every vertex of a v-vertex simple graph G with at least three vertices has degree at least $v/2$, then G has a Hamiltonian cycle.

8. (Ore's Theorem) If G is a v-vertex simple graph with $v \geq 3$ such that for each two non-adjacent vertices x and y the sum of the degrees of x and y is at least v, then G has a Hamiltonian cycle.

9. A question about whether a graph has a certain property is called a *graph decision problem.*

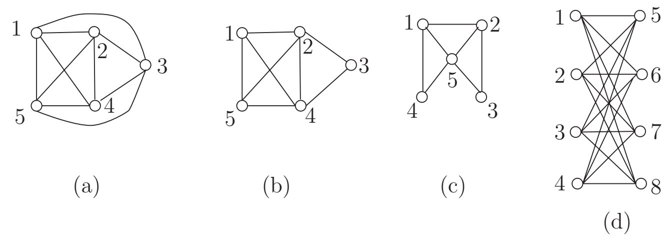
10. A **P**-*algorithm* or polynomial time algorithm for a property takes a graph as input and in time $O(n^k)$, where k is a positive integer independent of the input graph and n is a measure of the amount of information needed to specify the input graph, it outputs the answer "yes" if and only if the graph does have the property. We say the algorithm *accepts* the graph if it answers yes.

11. We say a property of graphs is *in the class* **P** if there is a **P**-algorithm that accepts exactly the graphs with the property.

12. An **NP**-algorithm (non-deterministic polynomial time) for a property takes a graph and $O(n^j)$ additional information, and in time $O(n^k)$, where k and j are positive integers independent of the the input graph and n is a measure of the amount of information needed to specify the input graph, outputs the answer yes if and only if it can use the additional information to determine that the graph has the property.

13. A graph decision problem in **NP** if called **NP**-complete if, for each other problem in **NP**, we can devise an algorithm for the second problem that has $O(n^k)$ steps (where n is a measure of the size of the input graph, and k is independent of n), including counting as one step solving an instance of the first problem, and accepts exactly the instances of the second problem that have a yes answer.

Figure 6.19: Some graphs

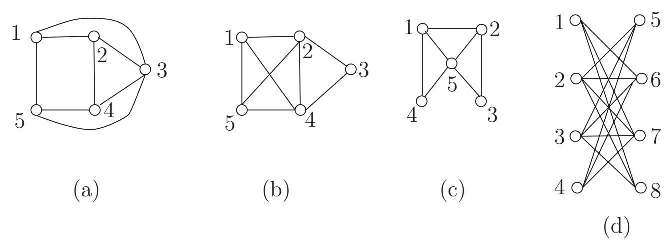


Problems

1. For each graph in Figure 6.19, either explain why the graph does not have an Eulerian circuit or find an Eulerian Circuit.

2. For each graph in Figure 6.20, either explain why the graph does not have an Eulerian Trail or find an Eulerian Trail.

Figure 6.20: Some more graphs



3. What is the minimum number of new bridges that would have to be built in Königsberg and where could they be built in order to give a graph with an Eulerian circuit?

4. If we built a new bridge in Königsberg between the Island and the top and bottom banks of the river, could we take a walk that crosses all the bridges and uses none twice? Either explain where could we start and end in that case or why we couldn't do it.

5. For which values of n does the complete graph on n vertices have an Eulerian Circuit?

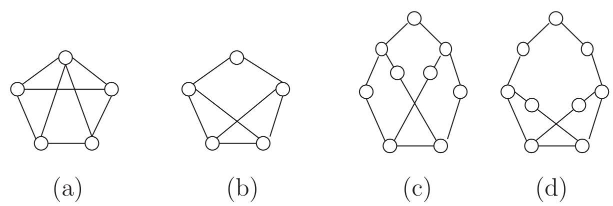
6. The hypercube graph Q_n has as its vertex set the n-tuples of zeros and ones. Two of these vertices are adjacent if and only if they are different in one position. The name comes from the fact that Q_3 can be drawn in three dimensional space as a cube. For what values of n is Q_n Eulerian?

7. For what values of n is the hypercube graph Q_n (see Problem 6) Hamiltonian?

8. Give an example of a graph which has a Hamiltonian cycle but no Eulerian Circuit and a graph which has an Eulerian Circuit but no Hamiltonian Cycle.

9. The complete bipartite graph $K_{m,n}$ is a graph with $m + n$ vertices. These vertices are divided into a set of size m and a set of size n. We call these sets the *parts* of the graph. Within each of these sets there are *no* edges. But between each pair of vertices in different sets, there is an edge. The graph $K_{4,4}$ is pictured in part (d) of Figure 6.19.
   (a) For what values of m and n is $K_{m,n}$ Eulerian?
   (b) For which values of m and n is $K_{m,n}$ Hamiltonian?
10. Show that the edge set of a graph in which each vertex has even degree may be partitioned into edge sets of cycles of the graph.
11. A cut-vertex of a graph is a vertex whose removal (along with all edges incident with it) increases the number of connected components of the graph. Describe any circumstances under which a graph with a cut vertex can be Hamiltonian.
12. Which of the graphs in Figure 6.21 satisfy the hypotheses of Dirac's Theorem? of Ore's Theorem? Which have Hamiltonian cycles?

Figure 6.21: Which of these graphs have Hamiltonian Cycles?



13. Prove Theorem 6.12.
14. The Hamiltonian Path problem is the problem of determining whether a graph has a Hamiltonian Path. Explain why this problem is in **NP**. Explain why the problem of determining whether a graph has a Hamiltonian Path is **NP**-complete.
15. The k-Path problem is the problem of determining whether a graph on n vertices has a path of length k, where k *is* allowed to depend on n. Show that the k-Path problem is **NP**-complete.
16. We form the Hamiltonian closure of a graph by constructing a sequence of graphs G_i with $G_0 = G$, and G_i formed from G_{i-1} by adding an edge between two nonadjacent vertices whose degree sum is at least nv. When we reach a G_i to which we cannot add such an edge, we call it a Hamiltonian Closure of G. Prove that a Hamiltonian Closure of a simple graph G is Hamiltonian if and only if G is.
17. Show that a simple connected graph has one and only one Hamiltonian closure.

6.4 Matching Theory

The idea of a matching

Suppose a school board is deciding among applicants for faculty positions. The school board has positions for teachers in a number of different grades, a position for an assistant librarian, two coaching positions, and for high school math and English teachers. They have many applicants, each of whom can fill more than one of the positions. They would like to know whether they can fill all the positions with people who have applied for jobs and have been judged as qualified.

Exercise 6.4-1 Table 6.1 shows a sample of the kinds of applications a school district might get for its positions. An x below an applicant's number means that that applicant qualifies for the position to the left of the x. Thus candidate 1 is qualified to teach second grade, third grade, and be an assistant librarian. The coaches teach physical education when they are not coaching, so a coach can't also hold one of the listed teaching positions. Draw a graph in which the vertices are labelled 1 through 9 for the applicants, and s, t, l, m, e, b, and f for the positions. Draw an edge from an applicant to a position if that applicant can fill that position. Use the graph to help you decide if it is possible to fill all the positions from among the applicants deemed suitable. If you can do so, give an assignment of people to jobs. If you cannot, try to explain why not.

Table 6.1: Some sample job application data

job\applicant	1	2	3	4	5	6	7	8	9
assistant librarian	x		x	x					
second grade	x	x	x	x					
third grade	x	x		x					
high school math				x	x	x			
high school English				x		x	x		
asst baseball coach						x	x	x	x
asst football coach					x	x		x	

Exercise 6.4-2 Table 6.2 shows a second sample of the kinds of applications a school district might get for its positions. Draw a graph as before and use it to help you decide if it is possible to fill all the positions from among the applicants deemed suitable. If you can do so, give an assignment of people to jobs. If you cannot, try to explain why not.

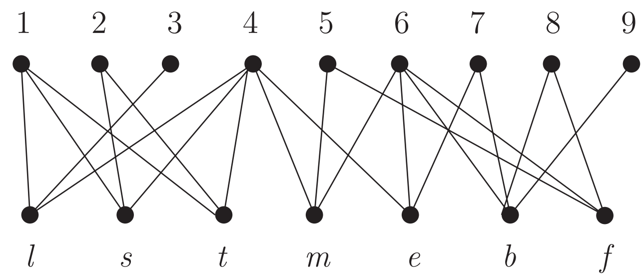
The graph of the data in Table 6.1 is shown in Figure 6.22.

From the figure it is clear that l:1, s:2, t:4, m:5, e:6, b:7, f:8 is one assignment of jobs to people that works. This assignment picks out a set of edges that share no endpoints. For example, the edge from l to 1 has no endpoint among s, t, m, e, b, f, 2, 3, 4, 5, 6, 7, or 8. A set of edges in a graph that share no endpoints is called a *matching* of the graph. Thus we have a matching between jobs and people that can fill the jobs. Since we don't want to assign two jobs to one

Table 6.2: Some other sample job application data

job\applicant	1	2	3	4	5	6	7	8	9
library assistant				x	x				
second grade	x	x	x					8	
third grade		x	x	x			x		x
high school math				x	x	x			
high school English					x	x			
asst baseball coach						x	x	x	x
asst football coach				x	x	x			

Figure 6.22: A graph of the data from Table 6.1.

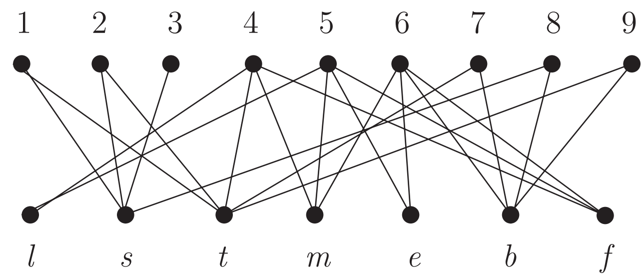


person or two people to one job, this is exactly the sort of solution we were looking for. Notice that the edge from l to 1 is a matching all by itself, so we weren't simply looking for a matching; we were looking for a matching that fills all the jobs. A matching is said to *saturate* a set X of vertices if every vertex in X is matched. We wanted a matching that saturates the jobs. In this case a matching that saturates all the jobs is a matching that is as big as possible, so it is also a *maximum* matching, that is, a matching that is at least as big as any other matching.

The graph in Figure 6.22 is an example of a "bipartite graph." A graph is called *bipartite* whenever its vertex set can be partitioned into two sets X and Y so that each edge connects a vertex in X with a vertex in Y. We can think of the jobs as the set X and the applicants as the set Y. Each of the two sets is called a *part* of the graph. A part of a bipartite graph is an example of an "independent set." A subset of the vertex set of a graph is called *independent* if no two of its vertices are joined by an edge. Thus a graph is bipartite if and only if its vertex set is a union of two independent sets. Notice that a bipartite graph cannot have any loop edges, because a loop would connect a vertex to a vertex in the same set. More generally, a vertex joined to itself by a loop cannot be in an independent set.

In a bipartite graph, it is sometimes easy to pick a maximum matching out just by staring at a drawing of the graph. However that is not always the case. Figure 6.23 is a graph of the data in Table 6.2. Staring at this Figure gives us many matchings, but no matching that saturates the set of jobs. But staring is not a proof, unless we can describe what we are staring at very well. Perhaps you tried to construct a matching by matching l to 4, s to 2, t to 7, m to 5, e to 6, b to 7, and then were frustrated when you got to f and 4, 5 and 6 were already used. You may then have gone back and tried to redo your earlier choices so as to keep one of 4, 5, or 6 free, and found you couldn't do so. This is because jobs l, m, e, and f are adjacent only to people 4, 5,

Figure 6.23: A graph of the data of Table 6.2.



and 6. Thus there are only three people qualified for these four jobs, and so there is no way we can fill them all.

We call the set $N(S)$ of all vertices adjacent to at least one vertex of S the *neighborhood* of S or the *neighbors* of S. In these terms, there is no matching that saturates a part X of a bipartite graph if there is some subset S of X such that the set $N(S)$ of neighbors of S is smaller than S. We call the set $N(S)$ of all vertices adjacent to at least one vertex of S the *neighborhood* of S or the *neighbors* of S. In symbols, we can summarize as follows.

Lemma 6.13 *If we can find a subset S of a part X of a bipartite graph G such that $|N(S)| < |S|$, then there is no matching of G that saturates X.*

Proof: A matching that saturates X must saturate S. But if there is such a matching, each element of S must be matched to a different vertex, and this vertex cannot be in S since $S \subseteq X$. Therefore there are edges from vertices in S to at least $|S|$ different vertices not in S, so $|N(S)| > |S|$, a contradiction. Thus there is no such matching.■

This gives a proof that there is no matching that saturates all the jobs, so the matching that matches l to 4, s to 2, t to 7, m to 5, e to 6, b to 7 is a maximum matching for the graph in Figure 6.23.

Another method you may have used to prove that there is no larger matching than the one we found is the following. When we matched l to 4, we may have noted that 4 is an endpoint of quite a few edges. Then when we matched s to 2, we may have noted that s is an endpoint of quite a few edges, and so is t. In fact, 4, s, and t touch 12 edges of the graph, and there are only 23 edges in the graph. If we could find three more vertices that touch the remaining edges of the graph, we would have six vertices that among them are incident with every edge. A set of vertices such that at least one of them is incident with each edge of a graph G is called a *vertex cover of the edges* of G, or a *vertex cover* of G for short. What does this have to do with a matching? Each matching edge would have to touch one, or perhaps two of the vertices in a vertex cover of the edges. Thus the number of edges in a matching is always less than the number of vertices in a vertex cover of the edges of a graph. Thus if we can find a vertex cover of size six in our graph in Figure 6.23, we will know that there is no matching that saturates the set of jobs since there are seven jobs. For future reference, we state our result about the size of a matching and the size of a vertex cover as a lemma.

Lemma 6.14 *The size of a matching in a graph G is no more than the size of a vertex cover of G.*

Proof: Given in the preceding discussion.■

We have seen that 4, s, and t are good candidates for being members of a relatively small vertex cover of the graph in Figure 6.23, since they cover more than half the edges of the graph. Continuing through the edges we first examined, we see that m, 6, and b are good candidates for a small vertex cover as well. In fact, $\{4, s, t, m, 6, b\}$ do form a vertex cover. Since we have a vertex cover of size six, we know a maximum matching has size no more than six. Since we have already found a six-edge matching, that is a maximum matching. Therefore with the data in Table 6.2, it is not possible to fill all the jobs.

Making matchings bigger

Practical problems involving matchings will usually lead us to search for the largest possible matching in a graph. To see how to use a matching to create a larger one, we will assume we have two matchings of the same graph and see how they differ, especially how a larger one differs from a smaller one.

Exercise 6.4-3 In the graph G of Figure 6.22, let M_1 be the matching $\{l, 1\}$, $\{s, 2\}$, $\{t, 4\}$, $\{m, 5\}$, $\{e, 6\}$, $\{b, 9\}$, $\{f, 8\}$, and let M_2 be the matching $\{l, 4\}$, $\{s, 2\}$ $\{t, 1\}$, $\{m, 6\}$, $\{e, 7\}$ $\{b, 8\}$. Recall that for sets S_1 and S_2 the symmetric difference of S_1 and S_2, denoted by $S_1 \Delta S_2$ is $(S_1 \cup S_2) - (S_1 \cap S_2)$. Compute the set $M_1 \Delta M_2$ and draw the graph with the same vertex set as G and edge set $M_1 \Delta M_2$. Use different colors or textures for the edges from M_1 and M_2 so you can see their interaction. Describe the kinds of graphs you see as connected components as succinctly as possible.

Exercise 6.4-4 In Exercise 6.4-3, one of the connected components suggests a way to modify M_2 by removing one or more edges and substituting one or more edges from M_1 that will give you a larger matching M_2' related to M_2. In particular, this larger matching should saturate everything M_2 saturates and more. What is M_2' and what else does it saturate?

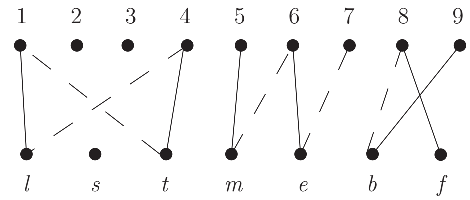
Exercise 6.4-5 Consider the matching $M = \{s, 1\}, \{t, 4\}, \{m, 6\}, \{b, 8\}$ in the graph of Figure 6.23. How does it relate to the simple path whose vertices are $3, s, 1, t, 4, m, 6, f$? Say as much as you can about the set M' that you obtain from M by deleting the edges of M that are in the path and adding to the result the edges of the path that are not in M.

In Exercise 6.4-3

$$M_1 \Delta M_2 = \{l, 1\}, \{l, 4\}, \{t, 4\}, \{t, 1\}, \{m, 5\}, \{m, 6\}, \{e, 6\}, \{e, 7\}, \{b, 8\}, \{f, 8\}, \{b, 9\}.$$

We have drawn the graph in Figure 6.24. We show the edges of M_2 as dashed. As you see, it consists of a cycle with four edges, alternating between edges of M_1 and M_2, a path with four edges, alternating between edges of M_1 and M_2, and a path with three edges, alternating between edges of M_1 and M_2. We call a simple path or cycle an *alternating path* or *alternating cycle* for a matching M of a graph G if its edges alternate between edges in M and edges not in M. Thus our connected components were alternating paths and cycles for both M_1 and M_2. The example we just discussed shows all the ways in which two matchings can differ in the following sense.

Figure 6.24: The graph for Exercise 6.4-3.



Lemma 6.15 (Berge) *If M_1 and M_2 are matchings of a graph $G = (V, E)$ then the connected components of $M_1 \Delta M_2$ are cycles with an even number of vertices and simple paths. Further, the cycles and paths are alternating cycles and paths for both M_1 and M_2.*

Proof: Each vertex of the graph $(V, M_1\Delta M_2)$ has degree 0, 1, or two. If a component has no cycles it is a tree, and the only kind of tree that has vertices of degree 1 and two is a simple path. If a component has a cycle, then it cannot have any edges other than the edges of the cycle incident with its vertices because the graph would then have a vertex of degree 3 or more. Thus the component must be a cycle. If two edges of a path or cycle in $(V, M_1\Delta M_2)$ share a vertex, they cannot come from the same matching, since two edges in the same matching do not share a vertex. Thus alternating edges of a path or cycle of $(V, M_1\Delta M_2)$ must come from different matchings. ■

Corollary 6.16 *If M_1 and M_2 are matchings of a graph $G = (V, E)$ and $|M_2| < |M_1|$, then there is an alternating path for M_1 and M_2 that starts and ends with vertices saturated by M_2 but not by M_1.*

Proof: Since an even alternating cycle and an even alternating path in $(V, M_1\Delta M_2)$ have equal numbers of edges from M_1 and M_2, at least one component must be an alternating path with more edges from M_1 than M_2, because otherwise $|M_2| \leq |M_1|$. Since this is a component of $(V, M_1\Delta M_2)$, its endpoints lie only in edges of M_2, so they are saturated by M_2 but not M_1. ■

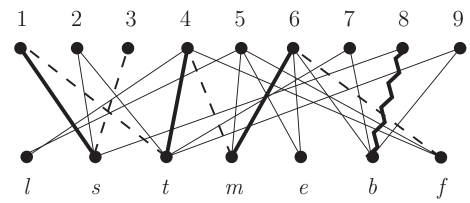
The path with three edges in Exercise 6.4-3 has two edges of M_1 and one edge of M_2. We see that if we remove $\{b, 8\}$ from M_2 and add $\{b, 9\}$ and $\{f, 8\}$, we get the matching

$$M_2' = \{\{l, 4\}, \{s, 2\}, \{t, 1\}, \{m, 6\}, \{e, 7\}, \{b, 9\}, \{f, 8\}\}.$$

This answers the question of Exercise 6.4-4. Notice that this matching saturates everything M_2 does, and also saturates vertices f and 9.

In Figure 6.25 we have shown the matching edges of the path in Exercise 6.4-5 in bold and the non-matching edges of the path as dashed. The edge of the matching not in the path is shown in zig-zag. Notice that the dashed edges and the zig-zag edge form a matching which is larger than M and saturates all the vertices that M does in addition to 3 and f. The path begins and ends with unmatched vertices, namely 3 and f, and and alternates between matching edges and non-matching edges. All but the first and last vertices of such a path lie on matching edges of the path and the endpoints of the path do not lie on matching edges. Thus no edges of the matching that are not path-edges will be incident with vertices on the path. Thus if we delete all the matching edges of the path from M and add all the other edges of the path to M, we will get

Figure 6.25: The path and matching of Exercise 6.4-5.



a new matching, because by taking every second edge of a simple path, we get edges that do not have endpoints in common. An alternating path is called an *augmenting path* for a matching M if it begins and ends with M-unsaturated vertices. That is, it is an alternating path that begins and ends with unmatched vertices. Our preceding discussion suggests the proof of the following theorem.

Theorem 6.17 (Berge) *A matching M in a graph is of maximum size if and only if M has no augmenting path. Further, if a matching M has an augmenting path P with edge set $E(P)$, then we can create a larger matching by deleting the edges in $M \cap E(P)$ from M and adding in the edges of $E(P) - M$.*

Proof: First if there is a matching M_1 larger than M, then by Corollary 6.16 there is an augmenting path for M. Thus if a matching has maximum size, it has no augmenting path. Further, as in our discussion of Exercise 6.4-5, if there is an augmenting path for M, then there is a larger matching for M. Finally, this discussion showed that if P is an augmenting path, we can get such a larger matching by deleting the edges in $M \cap E(P)$ and adding in the edges of $E(P) - M$. ■

Corollary 6.18 *While the larger matching of Theorem 6.17 may not contain M as a subset, it does saturate all the vertices that M saturates and two additional vertices.*

Proof: Every vertex incident with an edge in M is incident with some edge of the larger matching, and each of the two endpoints of the augmenting path is also incident with a matching edge. Because we may have removed edges of M to get the larger matching, it may not contain M.■

Matching in Bipartite Graphs

While our examples have all been bipartite, all our lemmas, corollaries and theorems about matchings have been about general graphs. In fact, it some of the results can be strengthened in bipartite graphs. For example, Lemma 6.14 tells us that the size of a matching is no more than the size of a vertex cover. We shall soon see that in a bipartite graph, the size of a maximum matching actually equals the size of a minimum vertex cover.

Searching for Augmenting Paths in Bipartite Graphs

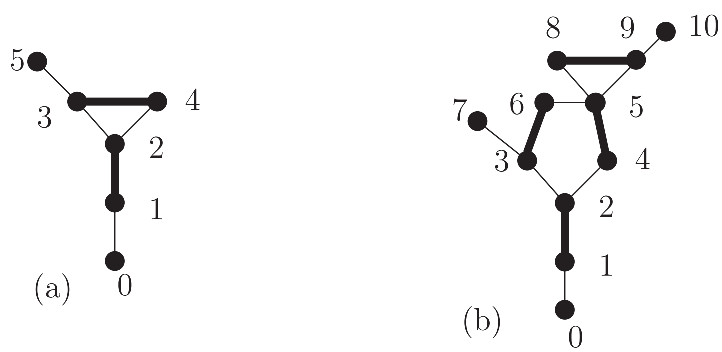
We have seen that if we can find an augmenting path for a matching M in a graph G, then we can create a bigger matching. Since our goal from the outset has been to create the largest matching possible, this helps us achieve that goal. However, you may ask, how do we find an augmenting path? Recall that a breadth-first search tree centered at a vertex x in a graph contains a path, in fact a shortest path, from x to every vertex y to which it is connected. Thus it seems that we ought to be able to alternate between matching edges and non-matching edges when doing a breadth-first search and find alternating paths. In particular, if we add vertex i to our tree by using a matching edge, then any edge we use to add a vertex *from* vertex i should be a non-matching edge. And if we add vertex i to our tree by using a non-matching edge, then any edge we use to add a vertex *from* vertex i should be a matching edge. (Thus there is just one such edge.) Because not all edges are available to us to use in adding vertices to the tree, the tree we get will not necessarily be a spanning tree of our original graph. However we can hope that if there is an augmenting path starting at vertex x and ending at vertex y, then we will find it by using breadth first search starting from x in this alternating manner.

Exercise 6.4-6 Given the matching $\{s, 2\}, \{t, 4\}, \{b, 7\}\{f, 8\}$ of the graph in Figure 6.22 use breadth-first search starting at vertex 1 in an alternating way to search for an augmenting path starting at vertex 1. Use the augmenting path you get to create a larger matching.

Exercise 6.4-7 Continue using the method of Exercise 6.4-6 until you find a matching of maximum size.

Exercise 6.4-8 Apply breadth-first search from vertex 0 in an alternating way to graph (a) in Figure 6.26. Does this method find an augmenting path? Is there an augmenting path?

Figure 6.26: Matching edges are shown in bold in these graphs.



For Exercise 6.4-6, if we begin at vertex 1, we add vertices l,s and t to our tree, giving them breadth-first numbers 1,2, and 3. Since l is not incident with a matching edge, we cannot continue the search from there. Since vertex s is incident with matching edge $\{s, 2\}$, we can use this edge to add vertex 2 to the tree and give it breadth-first number 4. This is the only vertex we can add from l since we can only use matching edges to add vertices from l. Similarly, from t we can add vertex 4 by using the matching edge $\{t, 4\}$ and giving it breadth-first number 5. All vertices adjacent to vertex 2 have already been added to the tree, but from vertex 4 we can use non-matching edges to add vertices m and e to our tree, giving them breadth first numbers 6 and 7. Now we can only use matching edges to add vertices to the tree from m or e, but there are no matching edges incident with them, so our alternating search tree stops here. Since m and e are unmatched, we know we have a path in our tree from vertex 1 to vertex m and a path from vertex 1 to vertex e. The vertex sequence of the path from 1 to m is $1s2t4m$ Thus our matching becomes $\{1, s\}, \{2, t\}, \{4, m\}, \{b, 7\}, \{f, 8\}$.

For Exercise 6.4-7 find another unmatched vertex and repeat the search. Working from vertex l, say, we start a tree by using the edges $\{l, 1\}, \{l, 3\}, \{l, 4\}$ to add vertices 1, 3, and 4. We could continue working on the tree, but since we see that $l\{l, 3\}3$ is an augmenting path, we use it to add the edge $\{l, 3\}$ to the matching, short-circuiting the tree-construction process. Thus our matching becomes $\{1, s\}, \{2, t\}, \{l, 3\}, \{4, m\}, \{b, 7\}\{f, 8\}$. The next unmatched vertex we see might be vertex 5. Starting from it, we add m and f to our tree, giving them breadth first numbers 1 and 2. From m we have the matching edge $\{m, 4\}$, and from f we have the matching edge $\{f, 8\}$, so we use them to add the vertices 4 and 8 to the tree. From vertex 4 we add l, s, t, and e to the tree, and from vertex 8 we add vertex b to the tree. All these vertices except e are in matching edges. Since e is not in a matching edge, we have discovered a vertex connected by an augmenting path to vertex 5. The path in the tree from vertex 5 to vertex e has vertex sequence $5m4e$, and using this augmenting path gives us the matching $\{1, s\}, \{2, t\}, \{l, 3\}, \{5, m\}, \{4, e\}, \{b, 7\}, \{f, 8\}$. Since we now have a matching whose size is the same as the size of a vertex cover, namely the bottom part of the graph in Figure 6.22, we have a matching of maximum size.

For Exercise 6.4-8 we start at vertex 0 and add vertex 1. From vertex 1 we use our matching edge to add vertex 2. From vertex 2 we use our two non-matching edges to add vertices 3 and 4. However, vertices 3 and 4 are incident with the same matching edge, so we cannot use that matching edge to add any vertices to the tree, and we must stop without finding an augmenting path. From staring at the picture, we see there is an augmenting path, namely 012435, and it gives us the matching $\{\{0, 1\}, \{2, 4\}, \{3, 5\}\}$. We would have similar difficulties in discovering either of the augmenting paths in part (b) of Figure 6.26.

It turns out to be the odd cycles in Figure 6.26 that prevent us from finding augmenting paths by our modification of breadth-first search. We shall demonstrate this by describing an algorithm which is a variation on the alternating breadth-first search we were using in solving our exercises. This algorithm takes a bipartite graph and a matching and either gives us an augmenting path or constructs a vertex cover whose size is the same as the size of the matching.

The Augmentation-Cover algorithm

We begin with a bipartite graph with parts X and Y and a matching M. We label the unmatched vertices in X with the label a (which stands for alternating). We number them in sequence as we label them. Starting with $i = 1$ and taking labeled vertices in order of the numbers we have assigned them, we use vertex number i to do additional labelling as follows.

1. If vertex i is in X, we label all unlabeled vertices adjacent to it with the label a and the name of vertex i. Then we number these newly labeled vertices, continuing our sequence of numbers without interruption.

2. If vertex i is in Y, and it is incident with an edge of M, its neighbor in the matching edge cannot yet be labeled. We label this neighbor with the label a and the name of vertex i.

3. If vertex i is in Y, and it is not incident with an edge of M, then we have discovered an augmenting path: the path from vertex i to the vertex we used to add it (and recorded at vertex i) and so on back to one of the unlabeled vertices in X. It is alternating by our labeling method, and it starts and ends with unsaturated vertices, so it is augmenting.

If we can continue the labelling process until no more labeling is possible and we do not find an augmenting path, then we let A be the set of labeled vertices. The set $C = (X - A) \cup (Y \cap A)$ then turns out to be a vertex cover whose size is the size of M. We call this algorithm the *augmentation-cover algorithm.*

Theorem 6.19 (König and Egerváry) *In a bipartite graph with parts X and Y, the size of a maximum sized matching equals the size of a minimum-sized vertex cover.*

Proof: In light of Berge's Theorem, if the augmentation-cover algorithm gives us an augmenting path, then the matching is not maximum sized, and in light of Lemma 6.14, if we can prove that the set C the algorithm gives us when there is no augmenting path is a vertex cover whose size is the size of the matching, we will have proved the theorem. To see that C is a vertex cover, note that every edge incident with a vertex in $X \cap A$ is covered, because its endpoint in Y has been marked with an a and so is in $Y \cap A$. But every other edge must be covered by $X - A$ because in a bipartite graph, each edge must be incident with a vertex in each part. Therefore C is a vertex cover. If an element of $Y \cap A$, were not matched, it would be an endpoint of an augmenting path, and so all elements of $Y \cap A$ are incident with matching edges. But every vertex of $X - A$ is matched because A includes all unmatched vertices of X. By step 2 of the augmentation-cover algorithm, if ϵ is a matching edge with an endpoint in $Y \cap A$, then the other endpoint must be in A. Therefore each matching edge contains only one member of C. Therefore the size of a maximum matching is the size of C. ■

Corollary 6.20 *The augmentation-cover algorithm applied to a bipartite graph and a matching of that graph produces either an augmenting path for the matching or a minimum vertex cover whose size equals the size of the matching.*

Before we proved the König-Egerváry Theorem, we knew that if we could find a matching and a vertex cover of the same size, then we had a maximum sized matching and a minimum sized vertex cover. However it is possible that in some graphs we can't test for whether a matching is as large as possible by comparing its size to that of a vertex cover because a maximum sized matching might be smaller than a minimum sized vertex cover. The König-Egárvary Theorem tells us that in bipartite graphs this problem never arises, so the test always works.

We had a second technique we used to show that a matching could not saturate the set X of all jobs in Exercise 6.4-2. In Lemma 6.13 we showed that if we can find a subset S of a part X of a bipartite graph G such that $|N(S)| < |S|$, then there is no matching of G that saturates X. In other words, to have a matching that saturates X in a bipartite graph on parts X and Y, it is necessary that $|N(S)| \geq |S|$ for *every* subset S of X. (When $S = \emptyset$, then so does $N(S)$.) This necessary condition is called *Hall's condition*, and Hall's theorem says that this necessary condition is sufficient.

Theorem 6.21 (Hall) *If G is a bipartite graph with parts X and Y, then there is a matching of G that saturates X if and only if $|N(S)| \geq |S|$ for every subset $\subseteq X$.*

Proof: In Lemma 6.13 we showed (the contrapositive of the statement) that if there is a matching of G, then $|N(S)| \geq |S|$ for every subset of X. (There is no reason to use a contrapositive argument though; if there is a matching that saturates X, then because matching edges have no endpoints in common, the elements of each subset S of X will be matched to at least $|S|$ different elements, and these will all be in $N(S)$.)

Thus we need only show that if the graph satisfies Hall's condition then there is a matching that saturates S. We will do this by showing that X is a minimum-sized vertex cover. Let C be some vertex cover of G. Let $S = X - C$. If ϵ is an edge from a vertex in S to a vertex $y \in Y$, ϵ cannot be covered by a vertex in $C \cap X$. Therefore ϵ must be covered by a vertex in $C \cap Y$. This means that $N(S) \subseteq C \cap Y$, so $|C \cap Y| \geq |N(S)|$. By Hall's condition, $N(S)| > |S|$. Therefore $|C \cap Y| \geq |S|$. Since $C \cap X$ and $C \cap Y$ are disjoint sets whose union is C, we can summarize our remarks with the equation

$$|C| = |C \cap X| + |C \cap Y| \geq |C \cap X| + |N(S)| \geq |C \cap X| + |S| = |C \cap X| + |C - X| = |X|.$$

X is a vertex cover, and we have just shown that it is a vertex cover of minimum size . Therefore a matching of maximum size has size $|X|$. Thus there is a matching that saturates X. ■

Good Algorithms

While Hall's theorem is quite elegant, applying it requires that we look at every subset of X, which would take us $\Omega\left(2^{|X|}\right)$ time. Similarly, actually finding a minimum vertex cover could involve looking at all (or nearly all) subsets of $X \cup Y$, which would also take us exponential time. However, the augmentation-cover algorithm requires that we examine each edge at most some fixed number of times and then do a little extra work; certainly no more than $O(e)$ work. We need to repeat the algorithm at most X times to find a maximum matching and minimum vertex cover. Thus in time $O(ev)$, we can not only find out whether we have a matching that saturates X; we can find such a matching if it exists and a vertex cover that proves it doesn't exist if it doesn't. However this only applies to bipartite graphs. The situation is much more complicated in non-bipartite graphs. In a paper which introduced the idea that a good algorithm is one that runs in time $O(n^c)$, where n is the amount of information needed to specify the input and c is a constant, Edmunds[10] developed a more complicated algorithm that extended the idea of a search tree to a more complicated structure he called a flower. He showed that this algorithm was good in his sense, introduced the problem class **NP**, and conjectured that $\mathbf{P} \neq \mathbf{NP}$. In a wry twist of fate, the problem of finding a minimum vertex cover problem (actually the problem of determining whether there is a vertex cover of size k, where k can be a function of v) is, in fact, **NP**-complete in arbitrary graphs. It is fascinating that the matching problem for general graphs turned out to be solvable in polynomial time, while determining the "natural" upper bound on the size of a matching, an upper bound that originally seemed quite useful, remains out of our reach.

[10] Jack Edmonds. Paths, Trees and Flowers. *Canadian Journal of Mathematics*, **17**, 1965 pp449-467

Important Concepts, Formulas, and Theorems

1. *Matching.* A set of edges in a graph that share no endpoints is called a *matching* of the graph.

2. *Saturate.* A matching is said to *saturate* a set X of vertices if every vertex in X is matched.

3. *Maximum Matching.* A matching in a graph is a *maximum matching* if it is at least as big as any other matching.

4. *Bipartite Graph.* A graph is called *bipartite* whenever its vertex set can be partitioned into two sets X and Y so that each edge connects a vertex in X with a vertex in Y. Each of the two sets is called a *part* of the graph.

5. *Independent Set.* A subset of the vertex set of a graph is called *independent* if no two of its vertices are connected by an edge. (In particular, a vertex connected to itself by a loop is in no independent set.) A part of a bipartite graph is an example of an 'independent set.

6. *Neighborhood.* We call the set $N(S)$ of all vertices adjacent to at least one vertex of S the *neighborhood* of S or the *neighbors* of S.

7. *Hall's theorem for a Matching in a Bipartite Graph.* If we can find a subset S of a part X of a bipartite graph G such that $|N(S)| < |S|$, then there is no matching of G that saturates X. If there is no subset $S \subseteq X$ such that $|N(S)| < |S|$, then there is a matching that saturates X.

8. *Vertex Cover.* A set of vertices such that at least one of them is incident with each edge of a graph G is called a *vertex cover of the edges* of G, or a *vertex cover* of G for short. In any graph, the size a matching is less than or equal to the size of any vertex cover.

9. *Alternating Path, Augmenting Path.* A simple path is called an *alternating path* for a matching M if, as we move along the path, the edges alternate between edges in M and edges not in M. An *augmenting path* is an alternating path that begins and ends at unmatched vertices.

10. *Berge's Lemma.* If M_1 and M_2 are matchings of a graph G then the connected components of $M_1 \Delta M_2$ are cycles with an even number of vertices and simple paths. Further, the cycles and paths are alternating cycles and paths for both M_1 and M_2.

11. *Berge's Corollary.* If M_1 and M_2 are matchings of a graph $G = (V, E)$ and $|M_1| > |M_2|$, then there is an alternating path for M_1 and M_2 that starts and ends with vertices saturated by M_1 but not by M_2.

12. *Berge's Theorem.* A matching M in a graph is of maximum size if and only if M has no augmenting path. Further, if a matching M has an augmenting path P with edge set $E(P)$, then we can create a larger matching by deleting the edges in $M \cap E(P)$ from M and adding in the edges of $E(P) - M$.

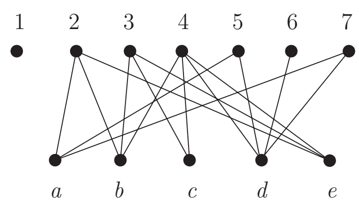
13. *Augmentation-Cover Algorithm.* The Augmentation-Cover algorithm is an algorithm that begins with a bipartite graph and a matching of that graph and produces either an augmenting path or a vertex cover whose size equals that of the matching, thus proving that the matching is a maximum matching.

14. *König-Egerváry Theorem.* In a bipartite graph with parts X and Y, the size of a maximum sized matching equals the size of a minimum-sized vertex cover.

Problems

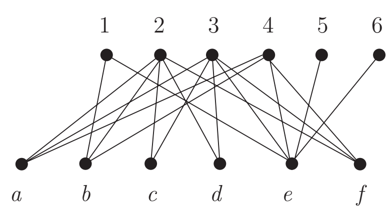
1. Either find a maximum matching or a subset S of the set $X = \{a, b, c, d, e\}$ such that $|S| > |N(S)|$ in the graph of Figure 6.27

Figure 6.27: A bipartite graph



2. Find a maximum matching and a minimum vertex cover in the graph of Figure 6.27
3. Either find a matching which saturates the set $X = \{a, b, c, d, e, f\}$ in Figure 6.28 or find a set S such that $|N(S)| < |X|$.

Figure 6.28: A bipartite graph



4. Find a maximum matching and a minimum vertex cover in the graph of Figure 6.28.
5. In the previous exercises, when you were able to find a set S with $|S| > |N(S)|$, how did $N(S)$ relate to the vertex cover? Why did this work out as it did?
6. A star is a another name for a tree with one vertex connected to each of n other vertices. (So a star has $n + 1$ vertices.) What are the size of a maximum matching and a minimum vertex cover in a star with $n + 1$ vertices?
7. In Theorem 6.17 is it true that if there is an augmenting path P with edge set $E(P)$ for a matching M, then $M \Delta E(P)$ is a larger matching than M?
8. Find a maximum matching and a minimum vertex cover in graph (b) of Figure 6.26.
9. In a bipartite graph, is one of the parts always a maximum-sized independent set? What if the graph is connected?

10. Find infinitely many examples of graphs in which a maximum-sized matching is smaller than a minimum-sized vertex cover.

11. Find an example of a graph in which the maximum size of a matching is less than one quarter of the size of a minimum vertex cover.

12. Prove or give a counter-example: Every tree is a bipartite graph. (Note, a single vertex with no edges is a bipartite graph; one of the two parts is empty.)

13. Prove or give a counter-example. A bipartite graph has no odd cycles.

14. Let G be a connected graph with no odd cycles. Let x be a vertex of G. Let X be all vertices at an even distance from x, and let Y be all vertices at an odd distance from x. Prove that G is bipartite with parts X and Y.

15. What is the sum of the maximum size of an independent set and the minimum size of a vertex cover in a graph G? Hint: it is useful to think both about the independent set and its complement (relative to the vertex set).

6.5 Coloring and planarity

The idea of coloring

Graph coloring was one of the origins of graph theory. It arose from a question from Francis Guthrie, who noticed that that four colors were enough colors to color the map of the counties of England so that if two counties shared a common boundary line, then they got different colors. He wondered whether this was the case for any map. Through his brother he passed it on to Agustus DeMorgan, and in this way it seeped into the consciousness of the mathematical community. If we think of the counties as vertices and draw an edge between two vertices if their counties share some boundary line, we get a representation of the problem that is independent of such things as the shape of the counties, the amount of boundary line they share, etc. so that it captures the part of the problem we need to focus on. We now color the vertices of the graph, and for this problem we want to do so in such a way that adjacent vertices get different colors. We will return to this problem later in the section; we begin our study with another application of coloring.

Exercise 6.5-1 The executive committee of the board of trustees of a small college has seven members, Kim, Smith, Jones, Gupta, Ramirez, Wang, and Chernov. It has six subcommittees with the following membership

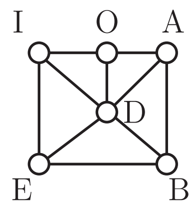
- Investments: W, R, G
- Operations: G, J, S, K
- Academic affairs: S, W, C
- Fund Raising: W, C, K
- Budget: G, R, C
- Enrollment: R, S, J, K

Each time the executive committee has a meeting, first each of the subcommittees meets with appropriate college officers, and then the executive committee gets together as a whole to go over subcommittee recommendations and make decisions. Two committees cannot meet at the same time if they have a member in common, but committees that don't have a member in common can meet at the same time. In this exercise you will figure out the minimum number of time slots needed to schedule all the subcommittee meetings. Draw a graph in which the vertices are named by the initials of the committee names and two vertices are adjacent if they have a member in common. Then assign numbers to the vertices in such a way that two adjacent vertices get different numbers. The numbers represent time slots, so they need not be distinct unless they are on adjacent vertices. What is the minimum possible number of numbers you need?

Because the problem of map coloring motivated much of graph theory, it is traditional to refer to the process of assigning labels to the vertices of a graph as coloring the graph. An assignment of labels, that is a function from the vertices to some set, is called a *coloring.* The set of possible labels (the range of the coloring function) is often referred to as a set of *colors.* Thus in Exercise 6.5-1 we are asking for a coloring of the graph. However, as with the map problem, we want a coloring in which adjacent vertices have different colors. A coloring of a graph is called a *proper coloring* if it assigns different colors to adjacent vertices.

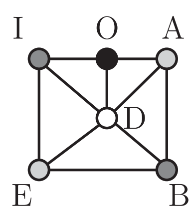
We have drawn the graph of Exercise 6.5-1 in Figure 6.29. We call this kind of graph an *intersection graph*, which means its vertices correspond to sets and it has an edge between two vertices if and only if the corresponding sets intersect.

Figure 6.29: The "intersection" graph of the committees.



The problem asked us to color the graph with as few colors possible, regarding the colors as 1,2,3, etc. We will represent 1 as a white vertex, 2 as a light grey vertex, 3 as a dark grey vertex and 4 as a black vertex. The triangle on the bottom requires three colors simply because all three vertices are adjacent. Since it doesn't matter which three colors we use, we choose arbitrarily to make them white, light grey, and dark grey. Now we know we need at least three colors to color the graph, so it makes sense to see if we can finish off a coloring using just three colors. Vertex I must be colored differently from E and D, so if we use the same three colors, it must have the same color as B. Similarly, vertex A would have to be the same color as E if we use the same three colors. But now none of the colors can be used on vertex O, because it is adjacent to three vertices of different colors. Thus we need at least four colors rather than 3, and we show a proper four-coloring in Figure 6.30.

Figure 6.30: A proper coloring of the committee intersection graph.



Exercise 6.5-2 How many colors are needed to give a proper coloring of the complete graph K_n?

Exercise 6.5-3 How many colors are needed for a proper coloring of a cycle C_n on $n = 3, 4, 5,$ and 6 vertices?

In Exercise 6.5-2 we need n colors to properly color K_n, because each pair of vertices is adjacent and thus must have two different colors. In Exercise 6.5-3, if n is even, we can just alternate two colors as we go around the cycle. However if n is odd, using two colors would require that they alternate as we go around the cycle, and when we colored our last vertex, it would be the same color as the first. Thus we need at least three colors, and by alternating two of them as we go around the cycle until we get to the last vertex and color it the third color we get a proper coloring with three colors.

The *chromatic number* of a graph G, traditionally denoted $\chi(G)$, is the minimum number of colors needed to properly color G. Thus we have shown that the chromatic number of the complete graph K_n is n, the chromatic number of a cycle on an even number of vertices is two, and the chromatic number of a cycle on an odd number of vertices is three. We showed that the chromatic number of our committee graph is 4.

From Exercise 6.5-2, we see that if a graph G has a subgraph which is a complete graph on n vertices, then we need at least n colors to color those vertices, so we need at least n colors to color G. this is useful enough that we will state it as a lemma.

Lemma 6.22 *If a graph G contains a subgraph that is a complete graph on n vertices, then the chromatic number of G is at least n.*

Proof: Given above.■

Interval Graphs

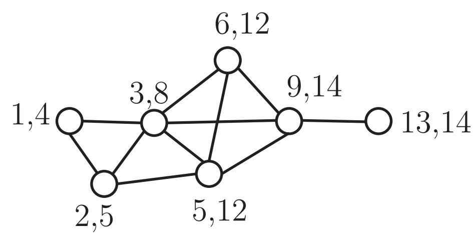
An interesting application of coloring arises in the design of optimizing compilers for computer languages. In addition to the usual RAM, a computer typically has some memory locations called registers which can be accessed at very high speeds. Thus values of variables which are going to be used again in the program are kept in registers if possible, so they will be quickly available when we need them. An optimizing compiler will attempt to decide the time interval in which a given variable may be used during a run of a program and arrange for that variable to be stored in a register for that entire interval of time. The time interval is not determined in absolute terms of seconds, but the relative endpoints of the intervals can be determined by when variables first appear and last appear as one steps through the computer code. This information is what is needed to set aside registers to use for the variables. We can think of coloring the variables by the registers as follows. We draw a graph in which the vertices are labeled with the variable names, and associated to each variable is the interval during which it is used. Two variables can use the same register if they are needed during non-overlapping time intervals. This is helpful, because registers are significantly more expensive than ordinary RAM, so they are limited in number. We can think of our graph on the variables as the intersection graph of the intervals. We want to color the graph properly with a minimum number of registers; hopefully this will be no more than the number of registers our computer has available. The problem of assigning variables to registers is called the *register assignment problem.*

An intersection graph of a set of intervals of real numbers is called an *interval graph.* The assignment of intervals to the vertices is called an *interval representation.* You will notice that so far in our discussion of coloring, we have not given an algorithm for properly coloring a graph efficiently. This is because the problem of whether a graph has a proper coloring with k colors, for any fixed k greater than 2 is another example of an **NP**-complete problem. However, for interval graphs, there is a very simple algorithm for properly coloring the graph in a minimum number of colors.

Exercise 6.5-4 Consider the closed intervals $[1, 4], [2, 5], [3, 8], [5, 12], [6, 12], [7, 14], [13, 14]$. Draw the interval graph determined by these intervals and find its chromatic number.

We have drawn the graph of Exercise 6.5-4 in Figure 6.31. (We have not included the square braces to avoid cluttering the figure.) Because of the way we have drawn it, it is easy to see a

Figure 6.31: The graph of Exercise 6.5-4



subgraph that is a complete graph on four vertices, so we know by our lemma that the graph has chromatic number at least four. In fact, Figure 6.32 shows that the chromatic number is exactly four. This is no accident.

Figure 6.32: A proper coloring of the graph of Exercise 6.5-4 with four colors

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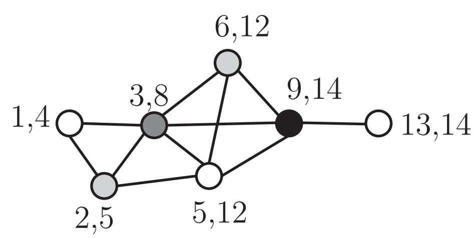


Theorem 6.23 *In an interval graph G, the chromatic number is the size of the largest complete subgraph.*

Proof: List the intervals of an interval representation of the graph in order of their left endpoints. Then color them with the integers 1 through some number n by starting with 1 on the first interval in the list and for each succeeding interval, use the smallest color not used on any neighbor of the interval earlier in the list. This will clearly give a proper coloring. To see that the number of colors needed is the size of the largest complete subgraph, let n denote the largest color used, and choose an interval I colored with color n. Then, by our coloring algorithm, I must intersect with earlier intervals in the list colored 1 through $n-1$; otherwise we could have used a smaller color on I. All these intervals must contain the left endpoint of I, because they intersect I and come earlier in the list. Therefore they all have a point in common, so they form a complete graph on n vertices. Therefore the minimum number of colors needed is the size of a complete subgraph of G. But by Lemma 6.22, G can have no larger complete subgraph. Thus the chromatic number of G is the size of the largest complete subgraph of G. ■

Corollary 6.24 *An interval graph G may be properly colored using $\chi(G)$ consecutive integers as colors by listing the intervals of a representation in order of their left endpoints and going through* *the list, assigning the smallest color not used on an earlier adjacent interval to each interval in the list.*

Proof: This is the coloring algorithm we used in the proof of Theorem 6.23. ■

Notice that using the correspondence between numbers and grey-shades we used before, the coloring in Figure 6.32 is the one given by this algorithm. An algorithm that colors an (arbitrary) graph G with consecutive integers by listing its vertices in some order, coloring the first vertex in the list 1, and then coloring each vertex with the least number not used on any adjacent vertices earlier in the list is called a *greedy coloring algorithm*. We have just seen that the greedy coloring algorithm allows us to find the chromatic number of an interval graph. This algorithm takes time $O(n^2)$, because as we go through the list, we might consider every earlier entry when we are considering a given element of the list. It is good luck that we have a polynomial time algorithm, because even though we stated in Theorem 6.23 that the chromatic number is the size of the largest complete subgraph, determining whether the size of a largest complete subgraph in a general graph (as opposed to an interval graph) is k (where k may be a function of the number of vertices) is an **NP-complete** problem.

Of course we assumed that we were given an interval representation of our graph. Suppose we are given a graph that happens to be an interval graph, but we don't know an interval representation. Can we still color it quickly? It turns out that there is a polynomial time algorithm to determine whether a graph is an interval graph and find an interval representation. This theory is quite beautiful,[11] but it would take us too far afield to pursue it now.

Planarity

We began our discussion of coloring with the map coloring problem. This problem has a special aspect that we did not mention. A map is drawn on a piece of paper, or on a globe. Thus a map is drawn either on the plane or on the surface of a sphere. By thinking of the sphere as a completely elastic balloon, we can imagine puncturing it with a pin somewhere where nothing is drawn, and then stretching the pinhole until we have the surface of the balloon laid out flat on a table. This means we can think of all maps as drawn in the plane. What does this mean about the graphs we associated with the maps? Say, to be specific, that we are talking about the counties of England. Then in each county we take an important town, and build a road to the boundary of each county with which it shares more than a single boundary point. We can build these roads so that they don't cross each other, and the roads to a boundary line between two different counties join together at that boundary line. Then the towns we chose are the vertices of a graph representing the map, and the roads are the edges. Thus given a map drawn in the plane, we can draw a graph to represent it in such a way that the edges of the graph do not meet at any point except their endpoints.[12] A graph is called *planar* if it has a drawing in the plane such that edges do not meet except at their endpoints. Such a drawing is called a *planar drawing* of the graph. The famous four color problem asked whether all planar graphs have proper four colorings. In 1976, Apel and Haken, building on some of the early attempts at proving the theorem, used a computer to demonstrate that four colors are sufficient to color

[11] See, for example, the book *Algorithmic Graph Theory and the Perfect Graph Conjecture*, by Martin Golumbic, Academic Press, New York, 1980.

[12] We are temporarily ignoring a small geographic feature of counties that we will mention when we have the terminology to describe it

any planar graph. While we do not have time to indicate how their proof went, there is now a book on the subject that gives a careful history of the problem and an explanation of what the computer was asked to do and why, assuming that the computer was correctly programmed, that led to a proof.[13]

What we will do here is derive enough information about planar graphs to show that five colors suffice, giving the student some background on planarity relevant to the design of computer chips.

We start out with two problems that aren't quite realistic, but are suggestive of how planarity enters chip design.

Exercise 6.5-5 A circuit is to be laid out on a computer chip in a single layer. The design includes five terminals (think of them as points to which multiple electrical circuits may be connected) that need to be connected so that it is possible for a current to go from any one of them to any other without sending current to a third. The connections are made with a narrow layer of metal deposited on the surface of the chip, which we will think of as a wire on the surface of the chip. Thus if one connection crosses another one, current in one wire will flow through the other as well. Thus the chip must be designed so that no two wires cross. Do you think this is possible?

Exercise 6.5-6 As in the previous exercise, we are laying out a computer circuit. However we now have six terminals, labeled a, b, c, 1, 2, and 3, such that each of a, b, and c must be connected to each of 1, 2, and 3, but there must be no other connections. As before, the wires cannot touch each other, so we need to design this chip so that no two wires cross. Do you think this is possible?

The answer to both these exercises is that it is not possible to design such a chip. One can make compelling geometric arguments why it is not possible, but they require that we visualize simultaneously a large variety of configurations with one picture. We will instead develop a few equations and inequalities relating to planar graphs that will allow us to give convincing arguments that both these designs are impossible.

The Faces of a Planar Drawing

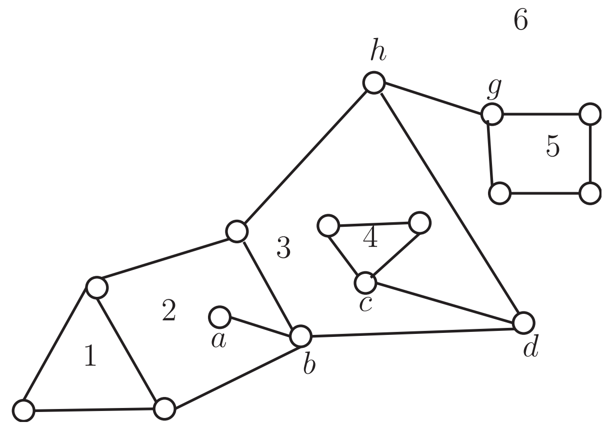
If we assume our graphs are finite, then it is easy to believe that we can draw any edge of a graph as a broken line segment (i.e. a bunch of line segments connected at their ends) rather than a smooth curve. In this way a cycle in our graph determines a polygon in our drawing. This polygon may have some of the graph drawn inside it and some of the graph drawn outside it. We say a subset of the plane is *geometrically connected* if between any two points of the region we can draw a curve.[14] (In our context, you may assume this curve is a broken line segment, but a careful study of geometric connectivity in general situations is less straightforward.) If we remove all the vertices and edges of the graph from the plane, we are likely to break it up into a number of connected sets.

Such a connected set is called a *face* of the drawing if it not a proper subset of any other connected set of the plane with the drawing removed. For example, in Figure 6.33 the faces are

[13] Robin Wilson, *Four Colors Suffice*. Princeton University Press, Princeton NJ 2003.

[14] The usual thing to say is that it is connected, but we want to distinguish this kind of connectivity form graphical connectivity. The fine point about counties that we didn't point out earlier is that they are geometrically connected. If they were not, the graph with a vertex for each county and an edge between two counties that share some boundary line would not necessarily be planar.

Figure 6.33: A typical graph and its faces.



marked 1, a triangular face, 2, a quadrilateral face that has a line segment and point removed for the edge $\{a, b\}$ and the vertex z, 3, another quadrilateral that now has not only a line but a triangle removed from it as well, 4, a triangular face, 5, a quadrilateral face, and 6 a face whose boundary is a heptagon connected by a line segment to a quadrilateral. Face 6 is called the "outside face" of the drawing and is the only face with infinite area. Each planar drawing of a graph will have an *outside face*, that is a face of infinite area in which we can draw a circle that encloses the entire graph. (Remember, we are thinking of our graphs as finite at this point.) Each edge either lies between two faces or has the same face on both its sides.The edges $\{a, b\}$, $\{c, d\}$ and $\{g, h\}$ are the edges of the second type. Thus if an edge lies on a cycle, it must divide two faces; otherwise removing that edge would increase the number of connected components of the graph. Such an edge is called a *cut edge* and cannot lie between two distinct faces. It is straightforward to show that any edge that is not a cut edge lies on a cycle. But if an edge lies on only one face, it is a cut edge, because we can draw a broken line segment from one side of the edge to the other, and this broken line segment plus part of the edge forms a closed curve that encloses part of the graph. Thus removing the edge disconnects the enclosed part of the graph from the rest of the graph.

Exercise 6.5-7 Draw some planar graphs with at least three faces and experiment to see if you can find a numerical relationship among v, the number of vertices, e, the number of edges, and f the number of faces. Check your relationship on the graph in Figure 6.33.

Exercise 6.5-8 In a simple graph, every face has at least three edges. This means that the number of pairs of a face and an edge bordering that face is at least $3f$. Use the fact that an edge borders either one or two faces to get an inequality relating the number of edges and the number of faces in a simple planar graph.

Some playing with planar drawings usually convinces people fairly quickly of the following theorem known as *Euler's Formula*.

Theorem 6.25 (Euler) *In a planar drawing of a graph G with v vertices, e edges, and f faces,*

$$v - e + f = 2.$$

Proof: We induct on the number of cycles of G. If G has no cycles, it is a tree, and a tree has one face because all its edges are cut-edges. Then $v - e + f = v - (v - 1) + 1 = 2$. Now suppose G has $n > 0$ cycles. Choose an edge which is between two faces, so it is part of a cycle. Deleting that edge joins the two faces it was on together, so the new graph has $f' = f - 1$ faces. The new graph has the same number of vertices and one less edge. It also has fewer cycles than G, so we have $v - (e - 1) - (f - 1) = 2$ by the inductive hypothesis, and this gives us $v - e + f = 2$. ■

ForExercise 6.5-8 let's define an edge-face pair to be an edge and a face such that the edge borders the face. Then we said that the number of such pairs is at least $3f$ in a simple graph. Since each edge is in either one or two faces, the number of edge-face pairs is also no more than $2e$. This gives us

$$3f \leq \# \text{ of edge-face pairs} \leq 2e,$$

or $3f \leq 2e$, so that $f \leq \frac{2}{3}e$ in a planar drawing of a graph. We can combine this with Theorem 6.25 to get

$$2 = v - e + f \leq v - e + \frac{2}{3}e = v - e/3$$

which we can rewrite as

$$e \leq 3v - 6$$

in a planar graph.

Corollary 6.26 *In a simple planar graph,* $e \leq 3v - 6$.

Proof: Given above.■

In our discussion of Exercise 6.5-5 we said that we would see a simple proof that the circuit layout problem was impossible. Notice that the question in that exercise was really the question of whether the complete graph on 5 vertices, K_5, is planar. If it were, the inequality $e \leq 3v - 6$ would give us $10 \leq 3 \cdot 5 - 6 = 9$, which is impossible, so K_5 can't be planar. The inequality of Corollary 6.26 is not strong enough to solve Exercise 6.5-6. This exercise is really asking whether the so-called "complete bipartite graph on two parts of size 3," denoted by $K_{3,3}$, is planar. In order to show that it isn't, we need to refine the inequality of Corollary 6.26 to take into account the fact that in a simple bipartite graph there are no cycles of size 3, so there are no faces that are bordered by just 3 edges. You are asked to do that in Problem 13.

Exercise 6.5-9 Prove or give a counter-example: Every planar graph has at least one vertex of degree 5 or less.

Exercise 6.5-10 Prove that every planar graph has a proper coloring with six colors.

In Exercise 6.5-9 suppose that G is a planar graph in which each vertex has degree six or more. Then the sum of the degrees of the vertices is at least 6v, and also is twice the number of edges. Thus $2e \geq 6v$, or $e \geq 3v$, contrary to $e \leq 3v - 6$. This gives us yet another corollary to Euler's formula.

Corollary 6.27 *Every planar graph has a vertex of degree 5 or less.*

Proof: Given above.■

The Five Color Theorem

We are now in a position to give a proof of the five color theorem, essentially Heawood's proof, which was based on his analysis of an incorrect proof given by Kempe to the four color theorem about ten years earlier in 1879. First we observe that in Exercise 6.5-10 we can use straightforward induction to show that any planar graph on n vertices can be properly colored in six colors. As a base step, the theorem is clearly true if the graph has six or fewer vertices. So now assume $n > 6$ and suppose that a graph with fewer than n vertices can be properly colored with six colors. Let x be a vertex of degree 5 or less. Deleting x gives us a planar graph on $n - 1$ vertices, so by the inductive hypothesis it can be properly colored with six colors. However only five or fewer of those colors can appear on vertices which were originally neighbors of x, because x had degree 5 or less. Thus we can replace x in the colored graph and there is at least one color not used on its neighbors. We use such a color on x and we have a proper coloring of G. Therefore, by the principle of mathematical induction, every planar graph on $n \geq 1$ vertices has a proper coloring with six colors.

To prove the five color theorem, we make a similar start. However, it is possible that after deleting x and using an inductive hypothesis to say that the resulting graph has a proper coloring with 5 colors, when we want to restore x into the graph, five distinct colors are already used on its neighbors. This is where the proof will become interesting.

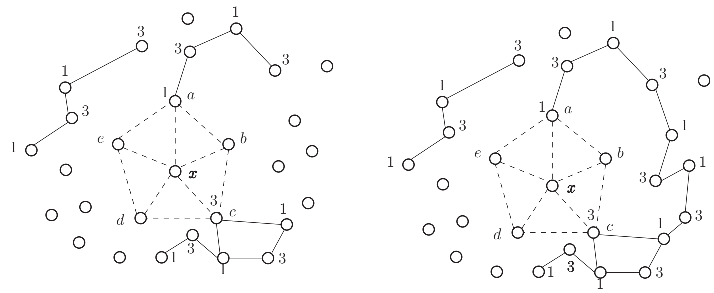
Theorem 6.28 *A planar graph G has a proper coloring with at most 5 colors.*

Proof: We may assume that every face except perhaps the outside face of our drawing is a triangle for two reasons. First, if we have a planar drawing with a face that is not a triangle, we can draw in additional edges going through that face until it has been divided into triangles, and the graph will remain planar. Second, if we can prove the theorem for graphs whose faces are all triangles, then we can obtain graphs with non-triangular faces by removing edges from graphs with triangular faces, and a proper coloring remains proper if we remove an edge from our graph. Although this appears to muddy the argument at this point, at a crucial point it makes it possible to give an argument that is clearer than it would otherwise be.

Our proof is by induction on the number of vertices of the graph. If G has five or fewer vertices then it is clearly properly colorable with five or fewer colors. Suppose G has n vertices and suppose inductively that every planar graph with fewer than n vertices is properly colorable with five colors. G has a vertex x of degree 5 or less. Let G' be the graph obtained by deleting x form G. By the inductive hypothesis, G' has a coloring with five or fewer colors. Fix such a coloring. Now if x has degree four or less, or if x has degree 5 but is adjacent to vertices colored with just four colors in G', then we may replace x in G' to get G and we have a color available to use on x to get a proper coloring of G.

Thus we may assume that x has degree 5, and that in G' five different colors appear on the vertices that are neighbors of x in G. Color all the vertices of G other than x as in G'. Let the five vertices adjacent to x be a, b, c, d, e in clockwise order, and assume they are colored with colors 1, 2, 3, 4, and 5. Further, by our assumption that all faces are triangles, we have that $\{a, b\}$, $\{b, c\}$4,{c,d},$\{d, e\}$, and $\{e, a\}$ are all edges, so that we have a pentagonal cycle surrounding x. Consider the graph $G_{1,3}$ of G which has the same vertex set as G but has only edges with endpoints colored 1 and 3. (Some possibilities are shown in Figure 6.34. We show only edges connecting vertices colored 1 and 3, as well as dashed lines for the edges from x to its neighbors and the edges between successive neighbors. There may be many more vertices and edges in G.)

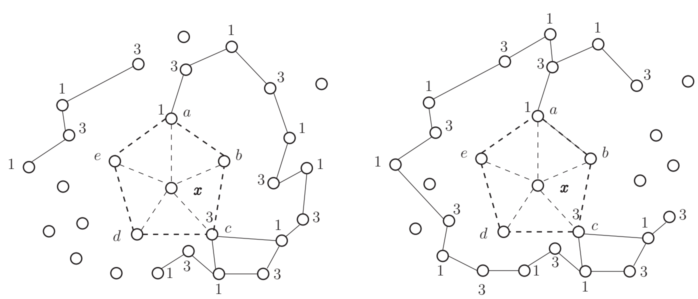
Figure 6.34: Some possibilities for the graph $G_{1,3}$.



The graph $G_{1,3}$ will have a number of connected components. If a and c are not in the same component, then we may exchange the colors on the vertices of the component containing a without affecting the color on c. In this way we obtain a coloring of G with only four colors, 3,2,3,4,5 on the vertices a, b, c, d, e. We may then use the fifth color (in this case 1) on vertex x and we have properly colored G with five colors.

Otherwise, as in the second part of Figure 6.34, since a and c are in the same component of $G_{1,3}$, there is a path from a to c consisting entirely of vertices colored 1 and 3. Now temporarily color x with a new color, say color 6. Then in G we have a cycle C of vertices colored 1, 3, and 6. This cycle has an inside and an outside. Part of the graph can be on the inside of C, and part can be on the outside. In Figure 6.35 we show two cases for how the cycle could occur, one in

Figure 6.35: Possible cycles in the graph $G_{1,3}$.



which vertex b is inside the cycle C and one in which it is outside C. (Notice also that in both cases, we have more than one choice for the cycle because there are two ways in which we could use the quadrilateral at the bottom of the figure.)

In G we also have the cycle with vertex sequence a, b, c, d, e which is colored with five different colors. This cycle and the cycle C can intersect only in the vertices a and c. Thus these two cycles divide the plane into four regions: the one inside both cycles, the one outside both cycles, and the two regions inside one cycle but not the other. If b is inside C, then the area inside both cycles is bounded by the cycle $a\{a, b\}b\{b, c\}c\{c, x\}x\{x, a\}a$. Therefore e and d are not inside the cycle

C. If one of d and e is inside C, then both are (because the edge between them cannot cross the cycle) and the boundary of the region inside both cycles is $a\{a,e\}e\{e,d\}d\{d,c\}c\{c,x\}x\{x,a\}a$. In this case b cannot be inside C. Therefore one of b and d is inside the cycle c and one is outside it. Therefore if we look at the graph $G_{2,4}$ with the same vertex set as G and just the edges connecting vertices colored 2 and 4, the connected component containing b and the connected component containing d must be different, because otherwise a path of vertices colored 2 and 4 would have to cross the cycle C colored with colors 1, 3, and 6. Therefore in G' we may exchange the colors 2 and 4 in the component containing d, and we now have only colors 1, 2, 3, and 5 used on vertices a, b, c, d, and e. Therefore we may use this coloring of G' as the coloring for the vertices of G different from x and we may change the color on x from 6 to 4, and we have a proper five coloring of G. Therefore by the principle of mathematical induction, every finite planar graph has a proper coloring with 5 colors. ■

Kempe's argument that seemed to prove the four color theorem was similar to this, though where we had five distinct colors on the neighbors of x and sought to remove one of them, he had four distinct colors on the five neighbors of x and sought to remove one of them. He had a more complicated argument involving two cycles in place of our cycle C, and he missed one of the ways in which these two cycles can interact.

Important Concepts, Formulas, and Theorems

1. *Graph Coloring.* An assignment of labels to the vertices of a graph, that is a function from the vertices to some set, is called a *coloring* of the graph. The set of possible labels (the range of the coloring function) is often referred to as a set of *colors*.

2. *Proper Coloring.* A coloring of a graph is called a *proper coloring* if it assigns different colors to adjacent vertices.

3. *Intersection Graph.* We call a graph an *intersection graph* if its vertices correspond to sets and it has an edge between two vertices if and only if the corresponding sets intersect.

4. *Chromatic Number.* The *chromatic number* of a graph G, traditionally denoted $\chi(G)$, is the minimum number of colors needed to properly color G.

5. *Complete Subgraphs and Chromatic Numbers.* If a graph G contains a subgraph that is a complete graph on n vertices, then the chromatic number of G is at least n.

6. *Interval Graph.* An intersection graph of a set of intervals of real numbers is called an *interval graph.* The assignment of intervals to the vertices is called an *interval representation.*

7. *Chromatic Number of an Interval Graph.* In an interval graph G, the chromatic number is the size of the largest complete subgraph.

8. *Algorithm to Compute the Chromatic number and a proper coloring of an Interval Graph.* An interval graph G may be properly colored using $\chi(G)$ consecutive integers as colors by listing the intervals of a representation in order of their left endpoints and going through the list, assigning the smallest color not used on an earlier adjacent interval to each interval in the list.

9. *Planar Graph and Planar Drawing.* A graph is called *planar* if it has a drawing in the plane such that edges do not meet except at their endpoints. Such a drawing is called a *planar drawing* of the graph.

10. *Face of a Planar Drawing.* A geometrically connected connected subset of the plane with the vertices and edges of a planar graph taken away is called a *face* of the drawing if it not a proper subset of any other connected set of the plane with the drawing removed.

11. *Cut Edge.* An edge whose removal from a graph increases the number of connected components is called a *cut edge* of the graph. A cut edge of a planar graph lies on only one face of a planar drawing.

12. *Euler's Formula.* Euler's formula states that in a planar drawing of a graph with v vertices, e edges and f faces, $v - e + f = 2$. As a consequence, in a planar graph, $e \le 3v - 6$.

Problems

1. What is the minimum number of colors needed to properly color a path on n vertices if $n > 1$?

2. What is the minimum number of colors needed to properly color a bipartite graph with parts X and Y.

3. If a graph has chromatic number two, is it bipartite? Why or why not?

4. Prove that the chromatic number of a graph G is the maximum of the chromatic numbers of its components.

5. A *wheel* on n vertices consists of a cycle on $n-1$ vertices together with one more vertex, normally drawn inside the cycle, which is connected to every vertex of the cycle. What is the chromatic number of a wheel on 5 vertices? What is the chromatic number of a wheel on an odd number of vertices?

6. A *wheel* on n vertices consists of a cycle on $n-1$ vertices together with one more vertex, normally drawn inside the cycle, which is connected to every vertex of the cycle. What is the chromatic number of a wheel on 6 vertices? What is the chromatic number of a wheel on an even number of vertices?

7. The usual symbol for the maximum degree of any vertex in a graph is Δ. Show that the chromatic number of a graph is no more than $\Delta + 1$. (In fact Brooks proved that if G is not complete or an odd cycle, then $\chi(G) \le \Delta$. Though there are now many proofs of this fact, none are easy!)

8. Can an interval graph contain a cycle with four vertices and no other edges between vertices of the cycle?

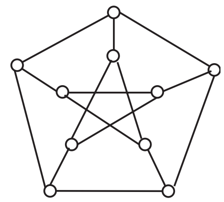
9. The Petersen graph is in Figure 6.36. What is its chromatic number?

10. Let G consist of a five cycle and a complete graph on four vertices, with all vertices of the five-cycle joined to all vertices of the complete graph. What is the chromatic number of G?

11. In how many ways can we properly color a tree on n vertices with t colors?

12. In how many ways may we properly color a complete graph on n vertices with t colors?

Figure 6.36: The Petersen Graph.



13. Show that in a simple planar graph with no triangles, $e \leq 2v - 4$.

14. Show that in a simple bipartite planar graph, $e \leq 2v - 4$, and use that fact to prove that $K_{3,3}$ is not planar.

15. Show that in a planar graph with no triangles there is a vertex of degree three or less.

16. Show that if a planar graph has fewer than twelve vertices, then it has at least one vertex of degree 4.

17. The Petersen Graph is in Figure 6.36. What is the size of the smallest cycle in the Petersen Graph? Is the Petersen Graph planar?

18. Prove the following Theorem of Welsh and Powell. If a graph G has degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$, then $\chi(G) \leq 1 + max_i[min(d_i, i-1)]$. (That is the maximum over all i of the minimum of d_i and $i - 1$.)

19. What upper bounds do Problem 18 and Problem 7 and the Brooks bound in Problem 7 give you for the chromatic number in Problem 10. Which comes closest to the right value? How close?

Index