VIII Appendix: Mathematical Background

Introduction

When we analyze algorithms, we often need to draw upon a body of mathematical tools. Some of these tools are as simple as high-school algebra, but others may be new to you. In Part I, we saw how to manipulate asymptotic notations and solve recurrences. This appendix comprises a compendium of several other concepts and methods we use to analyze algorithms. As noted in the introduction to Part I, you may have seen much of the material in this appendix before having read this book (although the specific notational conventions we use might occasionally differ from those you have seen elsewhere). Hence, you should treat this appendix as reference material. As in the rest of this book, however, we have included exercises and problems, in order for you to improve your skills in these areas.

Appendix A offers methods for evaluating and bounding summations, which occur frequently in the analysis of algorithms. Many of the formulas here appear in any calculus text, but you will find it convenient to have these methods compiled in one place.

Appendix B contains basic definitions and notations for sets, relations, functions, graphs, and trees. It also gives some basic properties of these mathematical objects.

Appendix C begins with elementary principles of counting: permutations, combinations, and the like. The remainder contains definitions and properties of basic probability. Most of the algorithms in this book require no probability for their analysis, and thus you can easily omit the latter sections of the chapter on a first reading, even without skimming them. Later, when you encounter a probabilistic analysis that you want to understand better, you will find Appendix C well organized for reference purposes.

Appendix D defines matrices, their operations, and some of their basic properties. You have probably seen most of this material already if you have taken a course in linear algebra, but you might find it helpful to have one place to look for our notation and definitions.

A Summations

When an algorithm contains an iterative control construct such as a **while** or **for** loop, we can express its running time as the sum of the times spent on each execution of the body of the loop. For example, we found in Section 2.2 that the jth iteration of insertion sort took time proportional to j in the worst case. By adding up the time spent on each iteration, we obtained the summation (or series)

$$\sum_{j=2}^{n} j \ .$$

When we evaluated this summation, we attained a bound of $\Theta(n^2)$ on the worst-case running time of the algorithm. This example illustrates why you should know how to manipulate and bound summations.

Section A.1 lists several basic formulas involving summations. Section A.2 offers useful techniques for bounding summations. We present the formulas in Section A.1 without proof, though proofs for some of them appear in Section A.2 to illustrate the methods of that section. You can find most of the other proofs in any calculus text.

A.1 Summation formulas and properties

Given a sequence $a_1, a_2, \ldots, a_n$ of numbers, where n is a nonnegative integer, we can write the finite sum $a_1 + a_2 + \cdots + a_n$ as

$$\sum_{k=1}^{n} a_k \ .$$

If $n = 0$, the value of the summation is defined to be 0. The value of a finite series is always well defined, and we can add its terms in any order.

Given an infinite sequence $a_1, a_2, \ldots$ of numbers, we can write the infinite sum $a_1 + a_2 + \cdots$ as

$$\sum_{k=1}^{\infty} a_k \ ,$$

which we interpret to mean

$$\lim_{n\to\infty} \sum_{k=1}^{n} a_k \ .$$

If the limit does not exist, the series ***diverges***; otherwise, it ***converges***. The terms of a convergent series cannot always be added in any order. We can, however, rearrange the terms of an ***absolutely convergent series***, that is, a series $\sum_{k=1}^{\infty} a_k$ for which the series $\sum_{k=1}^{\infty} |a_k|$ also converges.

Linearity

For any real number c and any finite sequences $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$,

$$\sum_{k=1}^{n} (ca_k + b_k) = c \sum_{k=1}^{n} a_k + \sum_{k=1}^{n} b_k \ .$$

The linearity property also applies to infinite convergent series.

We can exploit the linearity property to manipulate summations incorporating asymptotic notation. For example,

$$\sum_{k=1}^{n} \Theta(f(k)) = \Theta\left(\sum_{k=1}^{n} f(k)\right) \ .$$

In this equation, the Θ-notation on the left-hand side applies to the variable k, but on the right-hand side, it applies to n. We can also apply such manipulations to infinite convergent series.

Arithmetic series

The summation

$$\sum_{k=1}^{n} k = 1 + 2 + \cdots + n \ ,$$

is an ***arithmetic series*** and has the value

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

$$= \Theta(n^2) \ . \tag{A.2}$$

Sums of squares and cubes

We have the following summations of squares and cubes:

$$\sum_{k=0}^{n} k^2 = \frac{n(n+1)(2n+1)}{6}, \tag{A.3}$$

$$\sum_{k=0}^{n} k^3 = \frac{n^2(n+1)^2}{4}. \tag{A.4}$$

Geometric series

For real $x \neq 1$, the summation

$$\sum_{k=0}^{n} x^k = 1 + x + x^2 + \cdots + x^n$$

is a ***geometric*** or ***exponential series*** and has the value

$$\sum_{k=0}^{n} x^k = \frac{x^{n+1} - 1}{x - 1}. \tag{A.5}$$

When the summation is infinite and $|x| < 1$, we have the infinite decreasing geometric series

$$\sum_{k=0}^{\infty} x^k = \frac{1}{1 - x}. \tag{A.6}$$

Because we assume that $0^0 = 1$, these formulas apply even when $x = 0$.

Harmonic series

For positive integers n, the nth ***harmonic number*** is

$$\begin{aligned} H_n &= 1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \cdots + \frac{1}{n} \\ &= \sum_{k=1}^{n} \frac{1}{k} \\ &= \ln n + O(1). \end{aligned} \tag{A.7}$$

(We shall prove a related bound in Section A.2.)

Integrating and differentiating series

By integrating or differentiating the formulas above, additional formulas arise. For example, by differentiating both sides of the infinite geometric series (A.6) and multiplying by x, we get

$$\sum_{k=0}^{\infty} k x^k = \frac{x}{(1-x)^2} \tag{A.8}$$

for $|x| < 1$.

Telescoping series

For any sequence $a_0, a_1, \ldots, a_n$,

$$\sum_{k=1}^{n} (a_k - a_{k-1}) = a_n - a_0 \ , \tag{A.9}$$

since each of the terms $a_1, a_2, \ldots, a_{n-1}$ is added in exactly once and subtracted out exactly once. We say that the sum ***telescopes***. Similarly,

$$\sum_{k=0}^{n-1} (a_k - a_{k+1}) = a_0 - a_n \ .$$

As an example of a telescoping sum, consider the series

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

Since we can rewrite each term as

$$\frac{1}{k(k+1)} = \frac{1}{k} - \frac{1}{k+1} \ ,$$

we get

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

Products

We can write the finite product $a_1 a_2 \cdots a_n$ as

$$\prod_{k=1}^{n} a_k \ .$$

If $n = 0$, the value of the product is defined to be 1. We can convert a formula with a product to a formula with a summation by using the identity

$$\lg \left(\prod_{k=1}^{n} a_k \right) = \sum_{k=1}^{n} \lg a_k \ .$$

Exercises

A.1-1
Find a simple formula for $\sum_{k=1}^{n}(2k-1)$.

A.1-2 ⋆
Show that $\sum_{k=1}^{n} 1/(2k-1) = \ln(\sqrt{n}) + O(1)$ by manipulating the harmonic series.

A.1-3
Show that $\sum_{k=0}^{\infty} k^2 x^k = x(1+x)/(1-x)^3$ for $|x| < 1$.

A.1-4 ⋆
Show that $\sum_{k=0}^{\infty}(k-1)/2^k = 0$.

A.1-5 ⋆
Evaluate the sum $\sum_{k=1}^{\infty}(2k+1)x^{2k}$ for $|x| < 1$.

A.1-6
Prove that $\sum_{k=1}^{n} O(f_k(i)) = O\left(\sum_{k=1}^{n} f_k(i)\right)$ by using the linearity property of summations.

A.1-7
Evaluate the product $\prod_{k=1}^{n} 2 \cdot 4^k$.

A.1-8 ⋆
Evaluate the product $\prod_{k=2}^{n}(1-1/k^2)$.

A.2 Bounding summations

We have many techniques at our disposal for bounding the summations that describe the running times of algorithms. Here are some of the most frequently used methods.

Mathematical induction

The most basic way to evaluate a series is to use mathematical induction. As an example, let us prove that the arithmetic series $\sum_{k=1}^{n} k$ evaluates to $\frac{1}{2}n(n+1)$. We can easily verify this assertion for $n = 1$. We make the inductive assumption that

it holds for n, and we prove that it holds for $n + 1$. We have

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

You don't always need to guess the exact value of a summation in order to use mathematical induction. Instead, you can use induction to prove a bound on a summation. As an example, let us prove that the geometric series $\sum_{k=0}^{n} 3^k$ is $O(3^n)$. More specifically, let us prove that $\sum_{k=0}^{n} 3^k \le c3^n$ for some constant c. For the initial condition $n = 0$, we have $\sum_{k=0}^{0} 3^k = 1 \le c \cdot 1$ as long as $c \ge 1$. Assuming that the bound holds for n, let us prove that it holds for $n + 1$. We have

$$\begin{aligned}\sum_{k=0}^{n+1} 3^k &= \sum_{k=0}^{n} 3^k + 3^{n+1} \\ &\le c3^n + 3^{n+1} \qquad \text{(by the inductive hypothesis)} \\ &= \left(\frac{1}{3} + \frac{1}{c}\right) c3^{n+1} \\ &\le c3^{n+1}\end{aligned}$$

as long as $(1/3 + 1/c) \le 1$ or, equivalently, $c \ge 3/2$. Thus, $\sum_{k=0}^{n} 3^k = O(3^n)$, as we wished to show.

We have to be careful when we use asymptotic notation to prove bounds by induction. Consider the following fallacious proof that $\sum_{k=1}^{n} k = O(n)$. Certainly, $\sum_{k=1}^{1} k = O(1)$. Assuming that the bound holds for n, we now prove it for $n + 1$:

$$\begin{aligned}\sum_{k=1}^{n+1} k &= \sum_{k=1}^{n} k + (n+1) \\ &= O(n) + (n+1) \qquad \Longleftarrow \textit{wrong!!} \\ &= O(n+1) .\end{aligned}$$

The bug in the argument is that the "constant" hidden by the "big-oh" grows with n and thus is not constant. We have not shown that the same constant works for *all* n.

Bounding the terms

We can sometimes obtain a good upper bound on a series by bounding each term of the series, and it often suffices to use the largest term to bound the others. For

example, a quick upper bound on the arithmetic series (A.1) is

$$\begin{aligned}\sum_{k=1}^{n} k &\le \sum_{k=1}^{n} n \\ &= n^2 .\end{aligned}$$

In general, for a series $\sum_{k=1}^{n} a_k$, if we let $a_{\max} = \max_{1 \le k \le n} a_k$, then

$$\sum_{k=1}^{n} a_k \le n \cdot a_{\max} .$$

The technique of bounding each term in a series by the largest term is a weak method when the series can in fact be bounded by a geometric series. Given the series $\sum_{k=0}^{n} a_k$, suppose that $a_{k+1}/a_k \le r$ for all $k \ge 0$, where $0 < r < 1$ is a constant. We can bound the sum by an infinite decreasing geometric series, since $a_k \le a_0 r^k$, and thus

$$\begin{aligned}\sum_{k=0}^{n} a_k &\le \sum_{k=0}^{\infty} a_0 r^k \\ &= a_0 \sum_{k=0}^{\infty} r^k \\ &= a_0 \frac{1}{1-r} .\end{aligned}$$

We can apply this method to bound the summation $\sum_{k=1}^{\infty} (k/3^k)$. In order to start the summation at $k = 0$, we rewrite it as $\sum_{k=0}^{\infty} ((k+1)/3^{k+1})$. The first term ($a_0$) is $1/3$, and the ratio (r) of consecutive terms is

$$\begin{aligned}\frac{(k+2)/3^{k+2}}{(k+1)/3^{k+1}} &= \frac{1}{3} \cdot \frac{k+2}{k+1} \\ &\le \frac{2}{3}\end{aligned}$$

for all $k \ge 0$. Thus, we have

$$\begin{aligned}\sum_{k=1}^{\infty} \frac{k}{3^k} &= \sum_{k=0}^{\infty} \frac{k+1}{3^{k+1}} \\ &\le \frac{1}{3} \cdot \frac{1}{1-2/3} \\ &= 1 .\end{aligned}$$

A common bug in applying this method is to show that the ratio of consecutive terms is less than 1 and then to assume that the summation is bounded by a geometric series. An example is the infinite harmonic series, which diverges since

$$\begin{aligned}\sum_{k=1}^{\infty}\frac{1}{k} &= \lim_{n\to\infty}\sum_{k=1}^{n}\frac{1}{k}\\ &= \lim_{n\to\infty}\Theta(\lg n)\\ &= \infty\,.\end{aligned}$$

The ratio of the $(k+1)$st and kth terms in this series is $k/(k+1) < 1$, but the series is not bounded by a decreasing geometric series. To bound a series by a geometric series, we must show that there is an $r < 1$, which is a *constant*, such that the ratio of all pairs of consecutive terms never exceeds r. In the harmonic series, no such r exists because the ratio becomes arbitrarily close to 1.

Splitting summations

One way to obtain bounds on a difficult summation is to express the series as the sum of two or more series by partitioning the range of the index and then to bound each of the resulting series. For example, suppose we try to find a lower bound on the arithmetic series $\sum_{k=1}^{n} k$, which we have already seen has an upper bound of n^2. We might attempt to bound each term in the summation by the smallest term, but since that term is 1, we get a lower bound of n for the summation—far off from our upper bound of n^2.

We can obtain a better lower bound by first splitting the summation. Assume for convenience that n is even. We have

$$\begin{aligned}\sum_{k=1}^{n} k &= \sum_{k=1}^{n/2} k + \sum_{k=n/2+1}^{n} k\\ &\geq \sum_{k=1}^{n/2} 0 + \sum_{k=n/2+1}^{n} (n/2)\\ &= (n/2)^2\\ &= \Omega(n^2)\,,\end{aligned}$$

which is an asymptotically tight bound, since $\sum_{k=1}^{n} k = O(n^2)$.

For a summation arising from the analysis of an algorithm, we can often split the summation and ignore a constant number of the initial terms. Generally, this technique applies when each term a_k in a summation $\sum_{k=0}^{n} a_k$ is independent of n.

Then for any constant $k_0 > 0$, we can write

$$\begin{aligned}\sum_{k=0}^{n} a_k &= \sum_{k=0}^{k_0-1} a_k + \sum_{k=k_0}^{n} a_k \\ &= \Theta(1) + \sum_{k=k_0}^{n} a_k \ ,\end{aligned}$$

since the initial terms of the summation are all constant and there are a constant number of them. We can then use other methods to bound $\sum_{k=k_0}^{n} a_k$. This technique applies to infinite summations as well. For example, to find an asymptotic upper bound on

$$\sum_{k=0}^{\infty} \frac{k^2}{2^k} \ ,$$

we observe that the ratio of consecutive terms is

$$\begin{aligned}\frac{(k+1)^2/2^{k+1}}{k^2/2^k} &= \frac{(k+1)^2}{2k^2} \\ &\le \frac{8}{9}\end{aligned}$$

if $k \ge 3$. Thus, the summation can be split into

$$\begin{aligned}\sum_{k=0}^{\infty} \frac{k^2}{2^k} &= \sum_{k=0}^{2} \frac{k^2}{2^k} + \sum_{k=3}^{\infty} \frac{k^2}{2^k} \\ &\le \sum_{k=0}^{2} \frac{k^2}{2^k} + \frac{9}{8} \sum_{k=0}^{\infty} \left(\frac{8}{9}\right)^k \\ &= O(1) \ ,\end{aligned}$$

since the first summation has a constant number of terms and the second summation is a decreasing geometric series.

The technique of splitting summations can help us determine asymptotic bounds in much more difficult situations. For example, we can obtain a bound of $O(\lg n)$ on the harmonic series (A.7):

$$H_n = \sum_{k=1}^{n} \frac{1}{k} \ .$$

We do so by splitting the range 1 to n into $\lfloor \lg n \rfloor + 1$ pieces and upper-bounding the contribution of each piece by 1. For $i = 0, 1, \ldots, \lfloor \lg n \rfloor$, the ith piece consists

of the terms starting at $1/2^i$ and going up to but not including $1/2^{i+1}$. The last piece might contain terms not in the original harmonic series, and thus we have

$$\begin{aligned}\sum_{k=1}^{n}\frac{1}{k} &\le \sum_{i=0}^{\lfloor \lg n\rfloor}\sum_{j=0}^{2^i-1}\frac{1}{2^i+j}\\ &\le \sum_{i=0}^{\lfloor \lg n\rfloor}\sum_{j=0}^{2^i-1}\frac{1}{2^i}\\ &= \sum_{i=0}^{\lfloor \lg n\rfloor}1\\ &\le \lg n+1\,. \end{aligned} \tag{A.10}$$

Approximation by integrals

When a summation has the form $\sum_{k=m}^{n} f(k)$, where $f(k)$ is a monotonically increasing function, we can approximate it by integrals:

$$\int_{m-1}^{n} f(x)\,dx \le \sum_{k=m}^{n} f(k) \le \int_{m}^{n+1} f(x)\,dx\,. \tag{A.11}$$

Figure A.1 justifies this approximation. The summation is represented as the area of the rectangles in the figure, and the integral is the shaded region under the curve. When $f(k)$ is a monotonically decreasing function, we can use a similar method to provide the bounds

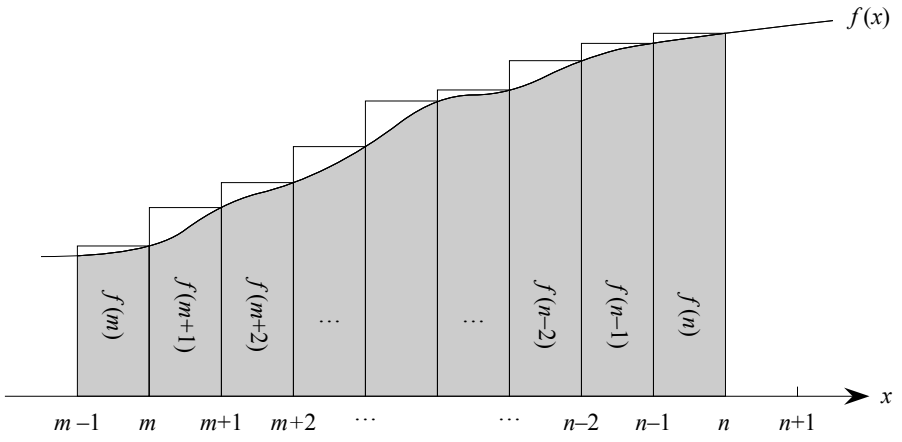
$$\int_{m}^{n+1} f(x)\,dx \le \sum_{k=m}^{n} f(k) \le \int_{m-1}^{n} f(x)\,dx\,. \tag{A.12}$$

The integral approximation (A.12) gives a tight estimate for the nth harmonic number. For a lower bound, we obtain

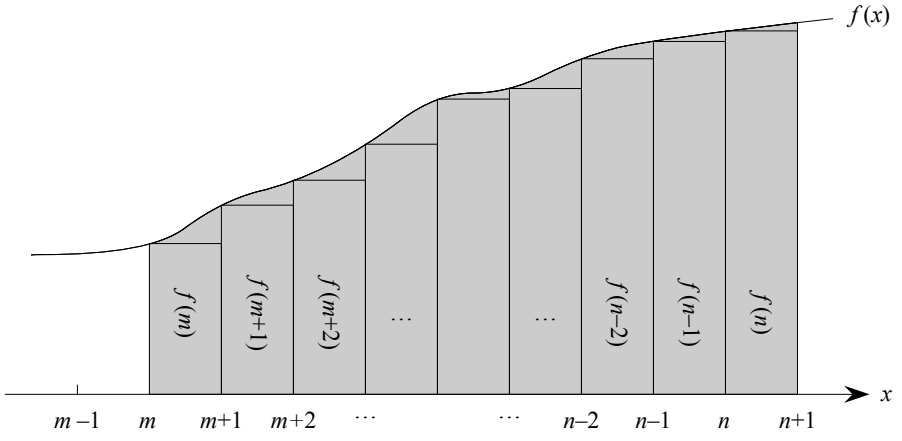
$$\begin{aligned}\sum_{k=1}^{n}\frac{1}{k} &\ge \int_{1}^{n+1}\frac{dx}{x}\\ &= \ln(n+1)\,. \end{aligned} \tag{A.13}$$

For the upper bound, we derive the inequality

$$\begin{aligned}\sum_{k=2}^{n}\frac{1}{k} &\le \int_{1}^{n}\frac{dx}{x}\\ &= \ln n\,, \end{aligned}$$



(a)



(b)

Figure A.1 Approximation of $\sum_{k=m}^{n} f(k)$ by integrals. The area of each rectangle is shown within the rectangle, and the total rectangle area represents the value of the summation. The integral is represented by the shaded area under the curve. By comparing areas in **(a)**, we get $\int_{m-1}^{n} f(x)\,dx \le \sum_{k=m}^{n} f(k)$, and then by shifting the rectangles one unit to the right, we get $\sum_{k=m}^{n} f(k) \le \int_{m}^{n+1} f(x)\,dx$ in **(b)**.

which yields the bound

$$\sum_{k=1}^{n} \frac{1}{k} \le \ln n + 1 \ . \tag{A.14}$$

Exercises

A.2-1
Show that $\sum_{k=1}^{n} 1/k^2$ is bounded above by a constant.

A.2-2
Find an asymptotic upper bound on the summation

$$\sum_{k=0}^{\lfloor \lg n \rfloor} \lceil n/2^k \rceil \ .$$

A.2-3
Show that the nth harmonic number is $\Omega(\lg n)$ by splitting the summation.

A.2-4
Approximate $\sum_{k=1}^{n} k^3$ with an integral.

A.2-5
Why didn't we use the integral approximation (A.12) directly on $\sum_{k=1}^{n} 1/k$ to obtain an upper bound on the nth harmonic number?

Problems

A-1 Bounding summations
Give asymptotically tight bounds on the following summations. Assume that $r \ge 0$ and $s \ge 0$ are constants.

a. $\displaystyle\sum_{k=1}^{n} k^r$.

b. $\displaystyle\sum_{k=1}^{n} \lg^s k$.

c. $\displaystyle\sum_{k=1}^{n} k^r \lg^s k$.

Appendix notes

Knuth [209] provides an excellent reference for the material presented here. You can find basic properties of series in any good calculus book, such as Apostol [18] or Thomas et al. [334].

B Sets, Etc.

Many chapters of this book touch on the elements of discrete mathematics. This appendix reviews more completely the notations, definitions, and elementary properties of sets, relations, functions, graphs, and trees. If you are already well versed in this material, you can probably just skim this chapter.

B.1 Sets

A ***set*** is a collection of distinguishable objects, called its ***members*** or ***elements***. If an object x is a member of a set S, we write $x \in S$ (read "x is a member of S" or, more briefly, "x is in S"). If x is not a member of S, we write $x \notin S$. We can describe a set by explicitly listing its members as a list inside braces. For example, we can define a set S to contain precisely the numbers 1, 2, and 3 by writing $S = \{1, 2, 3\}$. Since 2 is a member of the set S, we can write $2 \in S$, and since 4 is not a member, we have $4 \notin S$. A set cannot contain the same object more than once,[1] and its elements are not ordered. Two sets A and B are ***equal***, written $A = B$, if they contain the same elements. For example, $\{1, 2, 3, 1\} = \{1, 2, 3\} = \{3, 2, 1\}$.

We adopt special notations for frequently encountered sets:

- $\emptyset$ denotes the ***empty set***, that is, the set containing no members.
- $\mathbb{Z}$ denotes the set of ***integers***, that is, the set $\{\ldots, -2, -1, 0, 1, 2, \ldots\}$.
- $\mathbb{R}$ denotes the set of ***real numbers***.
- $\mathbb{N}$ denotes the set of ***natural numbers***, that is, the set $\{0, 1, 2, \ldots\}$.[2]

[1] A variation of a set, which can contain the same object more than once, is called a ***multiset***.

[2] Some authors start the natural numbers with 1 instead of 0. The modern trend seems to be to start with 0.

If all the elements of a set A are contained in a set B, that is, if $x \in A$ implies $x \in B$, then we write $A \subseteq B$ and say that A is a ***subset*** of B. A set A is a ***proper subset*** of B, written $A \subset B$, if $A \subseteq B$ but $A \neq B$. (Some authors use the symbol "$\subset$" to denote the ordinary subset relation, rather than the proper-subset relation.) For any set A, we have $A \subseteq A$. For two sets A and B, we have $A = B$ if and only if $A \subseteq B$ and $B \subseteq A$. For any three sets A, B, and C, if $A \subseteq B$ and $B \subseteq C$, then $A \subseteq C$. For any set A, we have $\emptyset \subseteq A$.

We sometimes define sets in terms of other sets. Given a set A, we can define a set $B \subseteq A$ by stating a property that distinguishes the elements of B. For example, we can define the set of even integers by $\{x : x \in \mathbb{Z} \text{ and } x/2 \text{ is an integer}\}$. The colon in this notation is read "such that." (Some authors use a vertical bar in place of the colon.)

Given two sets A and B, we can also define new sets by applying ***set operations***:

- The ***intersection*** of sets A and B is the set

  $$A \cap B = \{x : x \in A \text{ and } x \in B\} .$$

- The ***union*** of sets A and B is the set

  $$A \cup B = \{x : x \in A \text{ or } x \in B\} .$$

- The ***difference*** between two sets A and B is the set

  $$A - B = \{x : x \in A \text{ and } x \notin B\} .$$

Set operations obey the following laws:

Empty set laws:

$$\begin{aligned} A \cap \emptyset &= \emptyset , \\ A \cup \emptyset &= A . \end{aligned}$$

Idempotency laws:

$$\begin{aligned} A \cap A &= A , \\ A \cup A &= A . \end{aligned}$$

Commutative laws:

$$\begin{aligned} A \cap B &= B \cap A , \\ A \cup B &= B \cup A . \end{aligned}$$

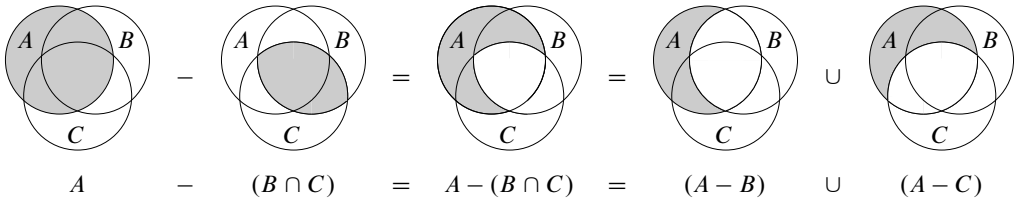


Figure B.1 A Venn diagram illustrating the first of DeMorgan's laws (B.2). Each of the sets A, B, and C is represented as a circle.

Associative laws:

$$\begin{aligned} A \cap (B \cap C) &= (A \cap B) \cap C \ , \\ A \cup (B \cup C) &= (A \cup B) \cup C \ . \end{aligned}$$

Distributive laws:

$$\begin{aligned} A \cap (B \cup C) &= (A \cap B) \cup (A \cap C) \ , \\ A \cup (B \cap C) &= (A \cup B) \cap (A \cup C) \ . \end{aligned} \tag{B.1}$$

Absorption laws:

$$\begin{aligned} A \cap (A \cup B) &= A \ , \\ A \cup (A \cap B) &= A \ . \end{aligned}$$

DeMorgan's laws:

$$\begin{aligned} A - (B \cap C) &= (A - B) \cup (A - C) \ , \\ A - (B \cup C) &= (A - B) \cap (A - C) \ . \end{aligned} \tag{B.2}$$

Figure B.1 illustrates the first of DeMorgan's laws, using a ***Venn diagram***: a graphical picture in which sets are represented as regions of the plane.

Often, all the sets under consideration are subsets of some larger set U called the ***universe***. For example, if we are considering various sets made up only of integers, the set $\mathbb{Z}$ of integers is an appropriate universe. Given a universe U, we define the ***complement*** of a set A as $\overline{A} = U - A = \{x : x \in U \text{ and } x \notin A\}$. For any set $A \subseteq U$, we have the following laws:

$$\begin{aligned} \overline{\overline{A}} &= A \ , \\ A \cap \overline{A} &= \emptyset \ , \\ A \cup \overline{A} &= U \ . \end{aligned}$$

We can rewrite DeMorgan's laws (B.2) with set complements. For any two sets $B, C \subseteq U$, we have

$$\begin{aligned}\overline{B \cap C} &= \overline{B} \cup \overline{C} \,, \\ \overline{B \cup C} &= \overline{B} \cap \overline{C} \,.\end{aligned}$$

Two sets A and B are ***disjoint*** if they have no elements in common, that is, if $A \cap B = \emptyset$. A collection $\mathcal{S} = \{S_i\}$ of nonempty sets forms a ***partition*** of a set S if

- the sets are ***pairwise disjoint***, that is, $S_i, S_j \in \mathcal{S}$ and $i \neq j$ imply $S_i \cap S_j = \emptyset$, and
- their union is S, that is,

$$S = \bigcup_{S_i \in \mathcal{S}} S_i \,.$$

In other words, $\mathcal{S}$ forms a partition of S if each element of S appears in exactly one $S_i \in \mathcal{S}$.

The number of elements in a set is the ***cardinality*** (or ***size***) of the set, denoted $|S|$. Two sets have the same cardinality if their elements can be put into a one-to-one correspondence. The cardinality of the empty set is $|\emptyset| = 0$. If the cardinality of a set is a natural number, we say the set is ***finite***; otherwise, it is ***infinite***. An infinite set that can be put into a one-to-one correspondence with the natural numbers $\mathbb{N}$ is ***countably infinite***; otherwise, it is ***uncountable***. For example, the integers $\mathbb{Z}$ are countable, but the reals $\mathbb{R}$ are uncountable.

For any two finite sets A and B, we have the identity

$$|A \cup B| = |A| + |B| - |A \cap B| \,, \tag{B.3}$$

from which we can conclude that

$$|A \cup B| \leq |A| + |B| \,.$$

If A and B are disjoint, then $|A \cap B| = 0$ and thus $|A \cup B| = |A| + |B|$. If $A \subseteq B$, then $|A| \leq |B|$.

A finite set of n elements is sometimes called an ***n-set***. A 1-set is called a ***singleton***. A subset of k elements of a set is sometimes called a ***k-subset***.

We denote the set of all subsets of a set S, including the empty set and S itself, by 2^S; we call 2^S the ***power set*** of S. For example, $2^{\{a,b\}} = \{\emptyset, \{a\}, \{b\}, \{a,b\}\}$. The power set of a finite set S has cardinality $2^{|S|}$ (see Exercise B.1-5).

We sometimes care about setlike structures in which the elements are ordered. An ***ordered pair*** of two elements a and b is denoted (a,b) and is defined formally as the set $(a,b) = \{a, \{a,b\}\}$. Thus, the ordered pair (a,b) is *not* the same as the ordered pair (b,a).

The ***Cartesian product*** of two sets A and B, denoted $A \times B$, is the set of all ordered pairs such that the first element of the pair is an element of A and the second is an element of B. More formally,

$$A \times B = \{(a, b) : a \in A \text{ and } b \in B\} .$$

For example, $\{a, b\} \times \{a, b, c\} = \{(a, a), (a, b), (a, c), (b, a), (b, b), (b, c)\}$. When A and B are finite sets, the cardinality of their Cartesian product is

$$|A \times B| = |A| \cdot |B| . \tag{B.4}$$

The Cartesian product of n sets $A_1, A_2, \ldots, A_n$ is the set of ***n-tuples***

$$A_1 \times A_2 \times \cdots \times A_n = \{(a_1, a_2, \ldots, a_n) : a_i \in A_i \text{ for } i = 1, 2, \ldots, n\} ,$$

whose cardinality is

$$|A_1 \times A_2 \times \cdots \times A_n| = |A_1| \cdot |A_2| \cdots |A_n|$$

if all sets are finite. We denote an n-fold Cartesian product over a single set A by the set

$$A^n = A \times A \times \cdots \times A ,$$

whose cardinality is $|A^n| = |A|^n$ if A is finite. We can also view an n-tuple as a finite sequence of length n (see page 1166).

Exercises

B.1-1
Draw Venn diagrams that illustrate the first of the distributive laws (B.1).

B.1-2
Prove the generalization of DeMorgan's laws to any finite collection of sets:

$$\begin{aligned} \overline{A_1 \cap A_2 \cap \cdots \cap A_n} &= \overline{A_1} \cup \overline{A_2} \cup \cdots \cup \overline{A_n} , \\ \overline{A_1 \cup A_2 \cup \cdots \cup A_n} &= \overline{A_1} \cap \overline{A_2} \cap \cdots \cap \overline{A_n} . \end{aligned}$$

B.1-3 ⋆
Prove the generalization of equation (B.3), which is called the ***principle of inclusion and exclusion***:

$$
\begin{aligned}
|A_1 \cup A_2 \cup \cdots \cup A_n| = \\
&|A_1| + |A_2| + \cdots + |A_n| \\
&- |A_1 \cap A_2| - |A_1 \cap A_3| - \cdots && \text{(all pairs)} \\
&+ |A_1 \cap A_2 \cap A_3| + \cdots && \text{(all triples)} \\
&\qquad\vdots \\
&+ (-1)^{n-1} |A_1 \cap A_2 \cap \cdots \cap A_n| \ .
\end{aligned}
$$

B.1-4
Show that the set of odd natural numbers is countable.

B.1-5
Show that for any finite set S, the power set 2^S has $2^{|S|}$ elements (that is, there are $2^{|S|}$ distinct subsets of S).

B.1-6
Give an inductive definition for an n-tuple by extending the set-theoretic definition for an ordered pair.

B.2 Relations

A ***binary relation*** R on two sets A and B is a subset of the Cartesian product $A \times B$. If $(a, b) \in R$, we sometimes write $a\ R\ b$. When we say that R is a binary relation on a set A, we mean that R is a subset of $A \times A$. For example, the "less than" relation on the natural numbers is the set $\{(a, b) : a, b \in \mathbb{N} \text{ and } a < b\}$. An n-ary relation on sets $A_1, A_2, \ldots, A_n$ is a subset of $A_1 \times A_2 \times \cdots \times A_n$.

A binary relation $R \subseteq A \times A$ is ***reflexive*** if

$a\ R\ a$

for all $a \in A$. For example, "$=$" and "$\leq$" are reflexive relations on $\mathbb{N}$, but "$<$" is not. The relation R is ***symmetric*** if

$a\ R\ b$ implies $b\ R\ a$

for all $a, b \in A$. For example, "$=$" is symmetric, but "$<$" and "$\leq$" are not. The relation R is ***transitive*** if

$a\ R\ b$ and $b\ R\ c$ imply $a\ R\ c$

for all $a, b, c \in A$. For example, the relations "$<$," "$\leq$," and "$=$" are transitive, but the relation $R = \{(a, b) : a, b \in \mathbb{N} \text{ and } a = b - 1\}$ is not, since $3\ R\ 4$ and $4\ R\ 5$ do not imply $3\ R\ 5$.

A relation that is reflexive, symmetric, and transitive is an ***equivalence relation***. For example, "$=$" is an equivalence relation on the natural numbers, but "$<$" is not. If R is an equivalence relation on a set A, then for $a \in A$, the ***equivalence class*** of a is the set $[a] = \{b \in A : a\ R\ b\}$, that is, the set of all elements equivalent to a. For example, if we define $R = \{(a, b) : a, b \in \mathbb{N} \text{ and } a + b \text{ is an even number}\}$, then R is an equivalence relation, since $a + a$ is even (reflexive), $a + b$ is even implies $b + a$ is even (symmetric), and $a + b$ is even and $b + c$ is even imply $a + c$ is even (transitive). The equivalence class of 4 is $[4] = \{0, 2, 4, 6, \ldots\}$, and the equivalence class of 3 is $[3] = \{1, 3, 5, 7, \ldots\}$. A basic theorem of equivalence classes is the following.

Theorem B.1 (An equivalence relation is the same as a partition)
The equivalence classes of any equivalence relation R on a set A form a partition of A, and any partition of A determines an equivalence relation on A for which the sets in the partition are the equivalence classes.

Proof For the first part of the proof, we must show that the equivalence classes of R are nonempty, pairwise-disjoint sets whose union is A. Because R is reflexive, $a \in [a]$, and so the equivalence classes are nonempty; moreover, since every element $a \in A$ belongs to the equivalence class $[a]$, the union of the equivalence classes is A. It remains to show that the equivalence classes are pairwise disjoint, that is, if two equivalence classes $[a]$ and $[b]$ have an element c in common, then they are in fact the same set. Suppose that $a\ R\ c$ and $b\ R\ c$. By symmetry, $c\ R\ b$, and by transitivity, $a\ R\ b$. Thus, for any arbitrary element $x \in [a]$, we have $x\ R\ a$ and, by transitivity, $x\ R\ b$, and thus $[a] \subseteq [b]$. Similarly, $[b] \subseteq [a]$, and thus $[a] = [b]$.

For the second part of the proof, let $\mathcal{A} = \{A_i\}$ be a partition of A, and define $R = \{(a, b) : \text{there exists } i \text{ such that } a \in A_i \text{ and } b \in A_i\}$. We claim that R is an equivalence relation on A. Reflexivity holds, since $a \in A_i$ implies $a\ R\ a$. Symmetry holds, because if $a\ R\ b$, then a and b are in the same set A_i, and hence $b\ R\ a$. If $a\ R\ b$ and $b\ R\ c$, then all three elements are in the same set A_i, and thus $a\ R\ c$ and transitivity holds. To see that the sets in the partition are the equivalence classes of R, observe that if $a \in A_i$, then $x \in [a]$ implies $x \in A_i$, and $x \in A_i$ implies $x \in [a]$. ■

A binary relation R on a set A is ***antisymmetric*** if

$a\ R\ b$ and $b\ R\ a$ imply $a = b$.

For example, the "$\leq$" relation on the natural numbers is antisymmetric, since $a \leq b$ and $b \leq a$ imply $a = b$. A relation that is reflexive, antisymmetric, and transitive is a ***partial order***, and we call a set on which a partial order is defined a ***partially ordered set***. For example, the relation "is a descendant of" is a partial order on the set of all people (if we view individuals as being their own descendants).

In a partially ordered set A, there may be no single "maximum" element a such that $b\ R\ a$ for all $b \in A$. Instead, the set may contain several ***maximal*** elements a such that for no $b \in A$, where $b \neq a$, is it the case that $a\ R\ b$. For example, a collection of different-sized boxes may contain several maximal boxes that don't fit inside any other box, yet it has no single "maximum" box into which any other box will fit.[3]

A relation R on a set A is a ***total relation*** if for all $a, b \in A$, we have $a\ R\ b$ or $b\ R\ a$ (or both), that is, if every pairing of elements of A is related by R. A partial order that is also a total relation is a ***total order*** or ***linear order***. For example, the relation "$\leq$" is a total order on the natural numbers, but the "is a descendant of" relation is not a total order on the set of all people, since there are individuals neither of whom is descended from the other. A total relation that is transitive, but not necessarily reflexive and antisymmetric, is a ***total preorder***.

Exercises

B.2-1

Prove that the subset relation "$\subseteq$" on all subsets of $\mathbb{Z}$ is a partial order but not a total order.

B.2-2

Show that for any positive integer n, the relation "equivalent modulo n" is an equivalence relation on the integers. (We say that $a \equiv b \pmod{n}$ if there exists an integer q such that $a - b = qn$.) Into what equivalence classes does this relation partition the integers?

B.2-3

Give examples of relations that are

a. reflexive and symmetric but not transitive,

b. reflexive and transitive but not symmetric,

c. symmetric and transitive but not reflexive.

---

[3] To be precise, in order for the "fit inside" relation to be a partial order, we need to view a box as fitting inside itself.

B.2-4
Let S be a finite set, and let R be an equivalence relation on $S \times S$. Show that if in addition R is antisymmetric, then the equivalence classes of S with respect to R are singletons.

B.2-5
Professor Narcissus claims that if a relation R is symmetric and transitive, then it is also reflexive. He offers the following proof. By symmetry, $a\ R\ b$ implies $b\ R\ a$. Transitivity, therefore, implies $a\ R\ a$. Is the professor correct?

B.3 Functions

Given two sets A and B, a ***function*** f is a binary relation on A and B such that for all $a \in A$, there exists precisely one $b \in B$ such that $(a, b) \in f$. The set A is called the ***domain*** of f, and the set B is called the ***codomain*** of f. We sometimes write $f : A \to B$; and if $(a, b) \in f$, we write $b = f(a)$, since b is uniquely determined by the choice of a.

Intuitively, the function f assigns an element of B to each element of A. No element of A is assigned two different elements of B, but the same element of B can be assigned to two different elements of A. For example, the binary relation

$$f = \{(a, b) : a, b \in \mathbb{N} \text{ and } b = a \bmod 2\}$$

is a function $f : \mathbb{N} \to \{0, 1\}$, since for each natural number a, there is exactly one value b in $\{0, 1\}$ such that $b = a \bmod 2$. For this example, $0 = f(0)$, $1 = f(1)$, $0 = f(2)$, etc. In contrast, the binary relation

$$g = \{(a, b) : a, b \in \mathbb{N} \text{ and } a + b \text{ is even}\}$$

is not a function, since $(1, 3)$ and $(1, 5)$ are both in g, and thus for the choice $a = 1$, there is not precisely one b such that $(a, b) \in g$.

Given a function $f : A \to B$, if $b = f(a)$, we say that a is the ***argument*** of f and that b is the ***value*** of f at a. We can define a function by stating its value for every element of its domain. For example, we might define $f(n) = 2n$ for $n \in \mathbb{N}$, which means $f = \{(n, 2n) : n \in \mathbb{N}\}$. Two functions f and g are ***equal*** if they have the same domain and codomain and if, for all a in the domain, $f(a) = g(a)$.

A ***finite sequence*** of length n is a function f whose domain is the set of n integers $\{0, 1, \ldots, n - 1\}$. We often denote a finite sequence by listing its values: $\langle f(0), f(1), \ldots, f(n - 1)\rangle$. An ***infinite sequence*** is a function whose domain is the set $\mathbb{N}$ of natural numbers. For example, the Fibonacci sequence, defined by recurrence (3.22), is the infinite sequence $\langle 0, 1, 1, 2, 3, 5, 8, 13, 21, \ldots\rangle$.

When the domain of a function f is a Cartesian product, we often omit the extra parentheses surrounding the argument of f. For example, if we had a function $f : A_1 \times A_2 \times \cdots \times A_n \to B$, we would write $b = f(a_1, a_2, \ldots, a_n)$ instead of $b = f((a_1, a_2, \ldots, a_n))$. We also call each a_i an ***argument*** to the function f, though technically the (single) argument to f is the n-tuple $(a_1, a_2, \ldots, a_n)$.

If $f : A \to B$ is a function and $b = f(a)$, then we sometimes say that b is the ***image*** of a under f. The image of a set $A' \subseteq A$ under f is defined by

$$f(A') = \{b \in B : b = f(a) \text{ for some } a \in A'\} .$$

The ***range*** of f is the image of its domain, that is, $f(A)$. For example, the range of the function $f : \mathbb{N} \to \mathbb{N}$ defined by $f(n) = 2n$ is $f(\mathbb{N}) = \{m : m = 2n \text{ for some } n \in \mathbb{N}\}$, in other words, the set of nonnegative even integers.

A function is a ***surjection*** if its range is its codomain. For example, the function $f(n) = \lfloor n/2 \rfloor$ is a surjective function from $\mathbb{N}$ to $\mathbb{N}$, since every element in $\mathbb{N}$ appears as the value of f for some argument. In contrast, the function $f(n) = 2n$ is not a surjective function from $\mathbb{N}$ to $\mathbb{N}$, since no argument to f can produce 3 as a value. The function $f(n) = 2n$ is, however, a surjective function from the natural numbers to the even numbers. A surjection $f : A \to B$ is sometimes described as mapping A ***onto*** B. When we say that f is onto, we mean that it is surjective.

A function $f : A \to B$ is an ***injection*** if distinct arguments to f produce distinct values, that is, if $a \neq a'$ implies $f(a) \neq f(a')$. For example, the function $f(n) = 2n$ is an injective function from $\mathbb{N}$ to $\mathbb{N}$, since each even number b is the image under f of at most one element of the domain, namely $b/2$. The function $f(n) = \lfloor n/2 \rfloor$ is not injective, since the value 1 is produced by two arguments: 2 and 3. An injection is sometimes called a ***one-to-one*** function.

A function $f : A \to B$ is a ***bijection*** if it is injective and surjective. For example, the function $f(n) = (-1)^n \lceil n/2 \rceil$ is a bijection from $\mathbb{N}$ to $\mathbb{Z}$:

$$\begin{aligned} 0 &\to 0 , \\ 1 &\to -1 , \\ 2 &\to 1 , \\ 3 &\to -2 , \\ 4 &\to 2 , \\ &\vdots \end{aligned}$$

The function is injective, since no element of $\mathbb{Z}$ is the image of more than one element of $\mathbb{N}$. It is surjective, since every element of $\mathbb{Z}$ appears as the image of some element of $\mathbb{N}$. Hence, the function is bijective. A bijection is sometimes called a ***one-to-one correspondence***, since it pairs elements in the domain and codomain. A bijection from a set A to itself is sometimes called a ***permutation***.

When a function f is bijective, we define its ***inverse*** f^{-1} as

$$f^{-1}(b) = a \text{ if and only if } f(a) = b .$$

For example, the inverse of the function $f(n) = (-1)^n \lceil n/2 \rceil$ is

$$f^{-1}(m) = \begin{cases} 2m & \text{if } m \geq 0\,, \\ -2m-1 & \text{if } m < 0\,. \end{cases}$$

Exercises

B.3-1
Let A and B be finite sets, and let $f : A \to B$ be a function. Show that

a. if f is injective, then $|A| \leq |B|$;

b. if f is surjective, then $|A| \geq |B|$.

B.3-2
Is the function $f(x) = x + 1$ bijective when the domain and the codomain are $\mathbb{N}$? Is it bijective when the domain and the codomain are $\mathbb{Z}$?

B.3-3
Give a natural definition for the inverse of a binary relation such that if a relation is in fact a bijective function, its relational inverse is its functional inverse.

B.3-4 ⋆
Give a bijection from $\mathbb{Z}$ to $\mathbb{Z} \times \mathbb{Z}$.

B.4 Graphs

This section presents two kinds of graphs: directed and undirected. Certain definitions in the literature differ from those given here, but for the most part, the differences are slight. Section 22.1 shows how we can represent graphs in computer memory.

A ***directed graph*** (or ***digraph***) G is a pair (V, E), where V is a finite set and E is a binary relation on V. The set V is called the ***vertex set*** of G, and its elements are called ***vertices*** (singular: ***vertex***). The set E is called the ***edge set*** of G, and its elements are called ***edges***. Figure B.2(a) is a pictorial representation of a directed graph on the vertex set $\{1, 2, 3, 4, 5, 6\}$. Vertices are represented by circles in the figure, and edges are represented by arrows. Note that ***self-loops***—edges from a vertex to itself—are possible.

In an ***undirected graph*** $G = (V, E)$, the edge set E consists of *unordered* pairs of vertices, rather than ordered pairs. That is, an edge is a set $\{u, v\}$, where

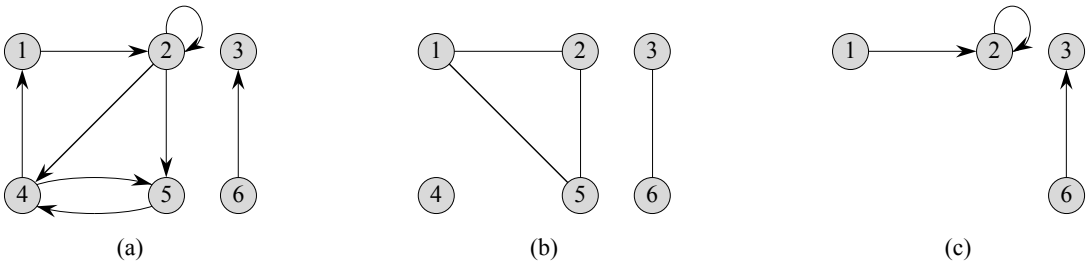


Figure B.2 Directed and undirected graphs. **(a)** A directed graph $G = (V, E)$, where $V = \{1, 2, 3, 4, 5, 6\}$ and $E = \{(1, 2), (2, 2), (2, 4), (2, 5), (4, 1), (4, 5), (5, 4), (6, 3)\}$. The edge $(2, 2)$ is a self-loop. **(b)** An undirected graph $G = (V, E)$, where $V = \{1, 2, 3, 4, 5, 6\}$ and $E = \{(1, 2), (1, 5), (2, 5), (3, 6)\}$. The vertex 4 is isolated. **(c)** The subgraph of the graph in part (a) induced by the vertex set $\{1, 2, 3, 6\}$.

$u, v \in V$ and $u \neq v$. By convention, we use the notation (u, v) for an edge, rather than the set notation $\{u, v\}$, and we consider (u, v) and (v, u) to be the same edge. In an undirected graph, self-loops are forbidden, and so every edge consists of two distinct vertices. Figure B.2(b) is a pictorial representation of an undirected graph on the vertex set $\{1, 2, 3, 4, 5, 6\}$.

Many definitions for directed and undirected graphs are the same, although certain terms have slightly different meanings in the two contexts. If (u, v) is an edge in a directed graph $G = (V, E)$, we say that (u, v) is ***incident from*** or ***leaves*** vertex u and is ***incident to*** or ***enters*** vertex v. For example, the edges leaving vertex 2 in Figure B.2(a) are $(2, 2)$, $(2, 4)$, and $(2, 5)$. The edges entering vertex 2 are $(1, 2)$ and $(2, 2)$. If (u, v) is an edge in an undirected graph $G = (V, E)$, we say that (u, v) is ***incident on*** vertices u and v. In Figure B.2(b), the edges incident on vertex 2 are $(1, 2)$ and $(2, 5)$.

If (u, v) is an edge in a graph $G = (V, E)$, we say that vertex v is ***adjacent*** to vertex u. When the graph is undirected, the adjacency relation is symmetric. When the graph is directed, the adjacency relation is not necessarily symmetric. If v is adjacent to u in a directed graph, we sometimes write $u \rightarrow v$. In parts (a) and (b) of Figure B.2, vertex 2 is adjacent to vertex 1, since the edge $(1, 2)$ belongs to both graphs. Vertex 1 is *not* adjacent to vertex 2 in Figure B.2(a), since the edge $(2, 1)$ does not belong to the graph.

The ***degree*** of a vertex in an undirected graph is the number of edges incident on it. For example, vertex 2 in Figure B.2(b) has degree 2. A vertex whose degree is 0, such as vertex 4 in Figure B.2(b), is ***isolated***. In a directed graph, the ***out-degree*** of a vertex is the number of edges leaving it, and the ***in-degree*** of a vertex is the number of edges entering it. The ***degree*** of a vertex in a directed graph is its in-

degree plus its out-degree. Vertex 2 in Figure B.2(a) has in-degree 2, out-degree 3, and degree 5.

A ***path*** of ***length*** k from a vertex u to a vertex u' in a graph $G = (V, E)$ is a sequence $\langle v_0, v_1, v_2, \ldots, v_k \rangle$ of vertices such that $u = v_0$, $u' = v_k$, and $(v_{i-1}, v_i) \in E$ for $i = 1, 2, \ldots, k$. The length of the path is the number of edges in the path. The path ***contains*** the vertices $v_0, v_1, \ldots, v_k$ and the edges $(v_0, v_1), (v_1, v_2), \ldots, (v_{k-1}, v_k)$. (There is always a 0-length path from u to u.) If there is a path p from u to u', we say that u' is ***reachable*** from u via p, which we sometimes write as $u \overset{p}{\rightsquigarrow} u'$ if G is directed. A path is ***simple*** [4]if all vertices in the path are distinct. In Figure B.2(a), the path $\langle 1, 2, 5, 4 \rangle$ is a simple path of length 3. The path $\langle 2, 5, 4, 5 \rangle$ is not simple.

A ***subpath*** of path $p = \langle v_0, v_1, \ldots, v_k \rangle$ is a contiguous subsequence of its vertices. That is, for any $0 \le i \le j \le k$, the subsequence of vertices $\langle v_i, v_{i+1}, \ldots, v_j \rangle$ is a subpath of p.

In a directed graph, a path $\langle v_0, v_1, \ldots, v_k \rangle$ forms a ***cycle*** if $v_0 = v_k$ and the path contains at least one edge. The cycle is ***simple*** if, in addition, $v_1, v_2, \ldots, v_k$ are distinct. A self-loop is a cycle of length 1. Two paths $\langle v_0, v_1, v_2, \ldots, v_{k-1}, v_0 \rangle$ and $\langle v'_0, v'_1, v'_2, \ldots, v'_{k-1}, v'_0 \rangle$ form the same cycle if there exists an integer j such that $v'_i = v_{(i+j) \bmod k}$ for $i = 0, 1, \ldots, k-1$. In Figure B.2(a), the path $\langle 1, 2, 4, 1 \rangle$ forms the same cycle as the paths $\langle 2, 4, 1, 2 \rangle$ and $\langle 4, 1, 2, 4 \rangle$. This cycle is simple, but the cycle $\langle 1, 2, 4, 5, 4, 1 \rangle$ is not. The cycle $\langle 2, 2 \rangle$ formed by the edge $(2, 2)$ is a self-loop. A directed graph with no self-loops is ***simple***. In an undirected graph, a path $\langle v_0, v_1, \ldots, v_k \rangle$ forms a ***cycle*** if $k > 0$, $v_0 = v_k$, and all edges on the path are distinct; the cycle is ***simple*** if $v_1, v_2, \ldots, v_k$ are distinct. For example, in Figure B.2(b), the path $\langle 1, 2, 5, 1 \rangle$ is a simple cycle. A graph with no simple cycles is ***acyclic***.

An undirected graph is ***connected*** if every vertex is reachable from all other vertices. The ***connected components*** of an undirected graph are the equivalence classes of vertices under the "is reachable from" relation. The graph in Figure B.2(b) has three connected components: $\{1, 2, 5\}$, $\{3, 6\}$, and $\{4\}$. Every vertex in $\{1, 2, 5\}$ is reachable from every other vertex in $\{1, 2, 5\}$. An undirected graph is connected if it has exactly one connected component. The edges of a connected component are those that are incident on only the vertices of the component; in other words, edge (u, v) is an edge of a connected component only if both u and v are vertices of the component.

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[4]Some authors refer to what we call a path as a "walk" and to what we call a simple path as just a "path." We use the terms "path" and "simple path" throughout this book in a manner consistent with their definitions.

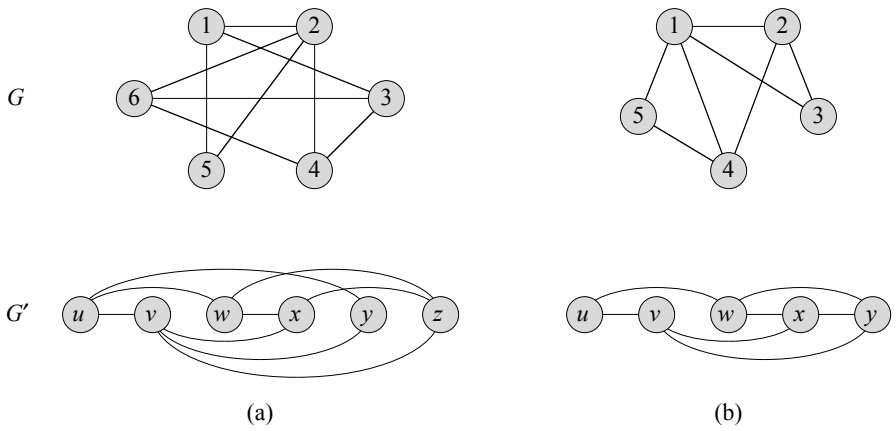

Figure B.3 **(a)** A pair of isomorphic graphs. The vertices of the top graph are mapped to the vertices of the bottom graph by $f(1) = u$, $f(2) = v$, $f(3) = w$, $f(4) = x$, $f(5) = y$, $f(6) = z$. **(b)** Two graphs that are not isomorphic, since the top graph has a vertex of degree 4 and the bottom graph does not.

A directed graph is ***strongly connected*** if every two vertices are reachable from each other. The ***strongly connected components*** of a directed graph are the equivalence classes of vertices under the "are mutually reachable" relation. A directed graph is strongly connected if it has only one strongly connected component. The graph in Figure B.2(a) has three strongly connected components: $\{1, 2, 4, 5\}$, $\{3\}$, and $\{6\}$. All pairs of vertices in $\{1, 2, 4, 5\}$ are mutually reachable. The vertices $\{3, 6\}$ do not form a strongly connected component, since vertex 6 cannot be reached from vertex 3.

Two graphs $G = (V, E)$ and $G' = (V', E')$ are ***isomorphic*** if there exists a bijection $f : V \to V'$ such that $(u, v) \in E$ if and only if $(f(u), f(v)) \in E'$. In other words, we can relabel the vertices of G to be vertices of G', maintaining the corresponding edges in G and G'. Figure B.3(a) shows a pair of isomorphic graphs G and G' with respective vertex sets $V = \{1, 2, 3, 4, 5, 6\}$ and $V' = \{u, v, w, x, y, z\}$. The mapping from V to V' given by $f(1) = u$, $f(2) = v$, $f(3) = w$, $f(4) = x$, $f(5) = y$, $f(6) = z$ provides the required bijective function. The graphs in Figure B.3(b) are not isomorphic. Although both graphs have 5 vertices and 7 edges, the top graph has a vertex of degree 4 and the bottom graph does not.

We say that a graph $G' = (V', E')$ is a ***subgraph*** of $G = (V, E)$ if $V' \subseteq V$ and $E' \subseteq E$. Given a set $V' \subseteq V$, the subgraph of G ***induced*** by V' is the graph $G' = (V', E')$, where

$$E' = \{(u, v) \in E : u, v \in V'\} \ .$$

The subgraph induced by the vertex set $\{1, 2, 3, 6\}$ in Figure B.2(a) appears in Figure B.2(c) and has the edge set $\{(1, 2), (2, 2), (6, 3)\}$.

Given an undirected graph $G = (V, E)$, the ***directed version*** of G is the directed graph $G' = (V, E')$, where $(u, v) \in E'$ if and only if $(u, v) \in E$. That is, we replace each undirected edge (u, v) in G by the two directed edges (u, v) and (v, u) in the directed version. Given a directed graph $G = (V, E)$, the ***undirected version*** of G is the undirected graph $G' = (V, E')$, where $(u, v) \in E'$ if and only if $u \neq v$ and E contains at least one of the edges (u, v) and (v, u). That is, the undirected version contains the edges of G "with their directions removed" and with self-loops eliminated. (Since (u, v) and (v, u) are the same edge in an undirected graph, the undirected version of a directed graph contains it only once, even if the directed graph contains both edges (u, v) and (v, u).) In a directed graph $G = (V, E)$, a ***neighbor*** of a vertex u is any vertex that is adjacent to u in the undirected version of G. That is, v is a neighbor of u if $u \neq v$ and either $(u, v) \in E$ or $(v, u) \in E$. In an undirected graph, u and v are neighbors if they are adjacent.

Several kinds of graphs have special names. A ***complete graph*** is an undirected graph in which every pair of vertices is adjacent. A ***bipartite graph*** is an undirected graph $G = (V, E)$ in which V can be partitioned into two sets V_1 and V_2 such that $(u, v) \in E$ implies either $u \in V_1$ and $v \in V_2$ or $u \in V_2$ and $v \in V_1$. That is, all edges go between the two sets V_1 and V_2. An acyclic, undirected graph is a ***forest***, and a connected, acyclic, undirected graph is a ***(free) tree*** (see Section B.5). We often take the first letters of "directed acyclic graph" and call such a graph a ***dag***.

There are two variants of graphs that you may occasionally encounter. A ***multigraph*** is like an undirected graph, but it can have both multiple edges between vertices and self-loops. A ***hypergraph*** is like an undirected graph, but each ***hyperedge***, rather than connecting two vertices, connects an arbitrary subset of vertices. Many algorithms written for ordinary directed and undirected graphs can be adapted to run on these graphlike structures.

The ***contraction*** of an undirected graph $G = (V, E)$ by an edge $e = (u, v)$ is a graph $G' = (V', E')$, where $V' = V - \{u, v\} \cup \{x\}$ and x is a new vertex. The set of edges E' is formed from E by deleting the edge (u, v) and, for each vertex w adjacent to u or v, deleting whichever of (u, w) and (v, w) is in E and adding the new edge (x, w). In effect, u and v are "contracted" into a single vertex.

Exercises

B.4-1

Attendees of a faculty party shake hands to greet each other, and each professor remembers how many times he or she shook hands. At the end of the party, the department head adds up the number of times that each professor shook hands.

Show that the result is even by proving the ***handshaking lemma***: if $G = (V, E)$ is an undirected graph, then

$$\sum_{v \in V} \text{degree}(v) = 2|E| \ .$$

B.4-2
Show that if a directed or undirected graph contains a path between two vertices u and v, then it contains a simple path between u and v. Show that if a directed graph contains a cycle, then it contains a simple cycle.

B.4-3
Show that any connected, undirected graph $G = (V, E)$ satisfies $|E| \geq |V| - 1$.

B.4-4
Verify that in an undirected graph, the "is reachable from" relation is an equivalence relation on the vertices of the graph. Which of the three properties of an equivalence relation hold in general for the "is reachable from" relation on the vertices of a directed graph?

B.4-5
What is the undirected version of the directed graph in Figure B.2(a)? What is the directed version of the undirected graph in Figure B.2(b)?

B.4-6 ⋆
Show that we can represent a hypergraph by a bipartite graph if we let incidence in the hypergraph correspond to adjacency in the bipartite graph. (*Hint:* Let one set of vertices in the bipartite graph correspond to vertices of the hypergraph, and let the other set of vertices of the bipartite graph correspond to hyperedges.)

B.5 Trees

As with graphs, there are many related, but slightly different, notions of trees. This section presents definitions and mathematical properties of several kinds of trees. Sections 10.4 and 22.1 describe how we can represent trees in computer memory.

B.5.1 Free trees

As defined in Section B.4, a ***free tree*** is a connected, acyclic, undirected graph. We often omit the adjective "free" when we say that a graph is a tree. If an undirected graph is acyclic but possibly disconnected, it is a ***forest***. Many algorithms that work

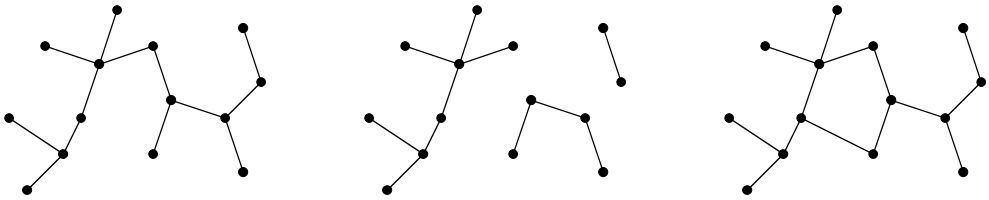

Figure B.4 **(a)** A free tree. **(b)** A forest. **(c)** A graph that contains a cycle and is therefore neither a tree nor a forest.

for trees also work for forests. Figure B.4(a) shows a free tree, and Figure B.4(b) shows a forest. The forest in Figure B.4(b) is not a tree because it is not connected. The graph in Figure B.4(c) is connected but neither a tree nor a forest, because it contains a cycle.

The following theorem captures many important facts about free trees.

Theorem B.2 (Properties of free trees)
Let $G = (V, E)$ be an undirected graph. The following statements are equivalent.

1. G is a free tree.
2. Any two vertices in G are connected by a unique simple path.
3. G is connected, but if any edge is removed from E, the resulting graph is disconnected.
4. G is connected, and $|E| = |V| - 1$.
5. G is acyclic, and $|E| = |V| - 1$.
6. G is acyclic, but if any edge is added to E, the resulting graph contains a cycle.

Proof (1) $\Rightarrow$ (2): Since a tree is connected, any two vertices in G are connected by at least one simple path. Suppose, for the sake of contradiction, that vertices u and v are connected by two distinct simple paths p_1 and p_2, as shown in Figure B.5. Let w be the vertex at which the paths first diverge; that is, w is the first vertex on both p_1 and p_2 whose successor on p_1 is x and whose successor on p_2 is y, where $x \neq y$. Let z be the first vertex at which the paths reconverge; that is, z is the first vertex following w on p_1 that is also on p_2. Let p' be the subpath of p_1 from w through x to z, and let p'' be the subpath of p_2 from w through y to z. Paths p' and p'' share no vertices except their endpoints. Thus, the path obtained by concatenating p' and the reverse of p'' is a cycle, which contradicts our assumption

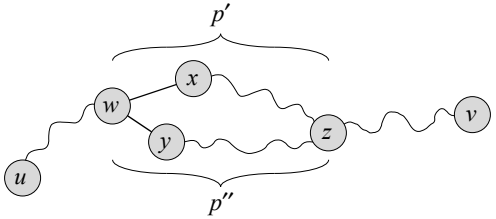

Figure B.5 A step in the proof of Theorem B.2: if (1) G is a free tree, then (2) any two vertices in G are connected by a unique simple path. Assume for the sake of contradiction that vertices u and v are connected by two distinct simple paths p_1 and p_2. These paths first diverge at vertex w, and they first reconverge at vertex z. The path p' concatenated with the reverse of the path p'' forms a cycle, which yields the contradiction.

that G is a tree. Thus, if G is a tree, there can be at most one simple path between two vertices.

(2) $\Rightarrow$ (3): If any two vertices in G are connected by a unique simple path, then G is connected. Let (u, v) be any edge in E. This edge is a path from u to v, and so it must be the unique path from u to v. If we remove (u, v) from G, there is no path from u to v, and hence its removal disconnects G.

(3) $\Rightarrow$ (4): By assumption, the graph G is connected, and by Exercise B.4-3, we have $|E| \geq |V| - 1$. We shall prove $|E| \leq |V| - 1$ by induction. A connected graph with $n = 1$ or $n = 2$ vertices has $n - 1$ edges. Suppose that G has $n \geq 3$ vertices and that all graphs satisfying (3) with fewer than n vertices also satisfy $|E| \leq |V| - 1$. Removing an arbitrary edge from G separates the graph into $k \geq 2$ connected components (actually $k = 2$). Each component satisfies (3), or else G would not satisfy (3). If we view each connected component V_i, with edge set E_i, as its own free tree, then because each component has fewer than $|V|$ vertices, by the inductive hypothesis we have $|E_i| \leq |V_i| - 1$. Thus, the number of edges in all components combined is at most $|V| - k \leq |V| - 2$. Adding in the removed edge yields $|E| \leq |V| - 1$.

(4) $\Rightarrow$ (5): Suppose that G is connected and that $|E| = |V| - 1$. We must show that G is acyclic. Suppose that G has a cycle containing k vertices $v_1, v_2, \ldots, v_k$, and without loss of generality assume that this cycle is simple. Let $G_k = (V_k, E_k)$ be the subgraph of G consisting of the cycle. Note that $|V_k| = |E_k| = k$. If $k < |V|$, there must be a vertex $v_{k+1} \in V - V_k$ that is adjacent to some vertex $v_i \in V_k$, since G is connected. Define $G_{k+1} = (V_{k+1}, E_{k+1})$ to be the subgraph of G with $V_{k+1} = V_k \cup \{v_{k+1}\}$ and $E_{k+1} = E_k \cup \{(v_i, v_{k+1})\}$. Note that $|V_{k+1}| = |E_{k+1}| = k + 1$. If $k + 1 < |V|$, we can continue, defining G_{k+2} in the same manner, and so forth, until we obtain $G_n = (V_n, E_n)$, where $n = |V|$,

$V_n = V$, and $|E_n| = |V_n| = |V|$. Since G_n is a subgraph of G, we have $E_n \subseteq E$, and hence $|E| \geq |V|$, which contradicts the assumption that $|E| = |V| - 1$. Thus, G is acyclic.

(5) $\Rightarrow$ (6): Suppose that G is acyclic and that $|E| = |V| - 1$. Let k be the number of connected components of G. Each connected component is a free tree by definition, and since (1) implies (5), the sum of all edges in all connected components of G is $|V| - k$. Consequently, we must have $k = 1$, and G is in fact a tree. Since (1) implies (2), any two vertices in G are connected by a unique simple path. Thus, adding any edge to G creates a cycle.

(6) $\Rightarrow$ (1): Suppose that G is acyclic but that adding any edge to E creates a cycle. We must show that G is connected. Let u and v be arbitrary vertices in G. If u and v are not already adjacent, adding the edge (u, v) creates a cycle in which all edges but (u, v) belong to G. Thus, the cycle minus edge (u, v) must contain a path from u to v, and since u and v were chosen arbitrarily, G is connected. ■

B.5.2 Rooted and ordered trees

A ***rooted tree*** is a free tree in which one of the vertices is distinguished from the others. We call the distinguished vertex the ***root*** of the tree. We often refer to a vertex of a rooted tree as a ***node***[5] of the tree. Figure B.6(a) shows a rooted tree on a set of 12 nodes with root 7.

Consider a node x in a rooted tree T with root r. We call any node y on the unique simple path from r to x an ***ancestor*** of x. If y is an ancestor of x, then x is a ***descendant*** of y. (Every node is both an ancestor and a descendant of itself.) If y is an ancestor of x and $x \neq y$, then y is a ***proper ancestor*** of x and x is a ***proper descendant*** of y. The ***subtree rooted at x*** is the tree induced by descendants of x, rooted at x. For example, the subtree rooted at node 8 in Figure B.6(a) contains nodes 8, 6, 5, and 9.

If the last edge on the simple path from the root r of a tree T to a node x is (y, x), then y is the ***parent*** of x, and x is a ***child*** of y. The root is the only node in T with no parent. If two nodes have the same parent, they are ***siblings***. A node with no children is a ***leaf*** or ***external node***. A nonleaf node is an ***internal node***.

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[5]The term "node" is often used in the graph theory literature as a synonym for "vertex." We reserve the term "node" to mean a vertex of a rooted tree.

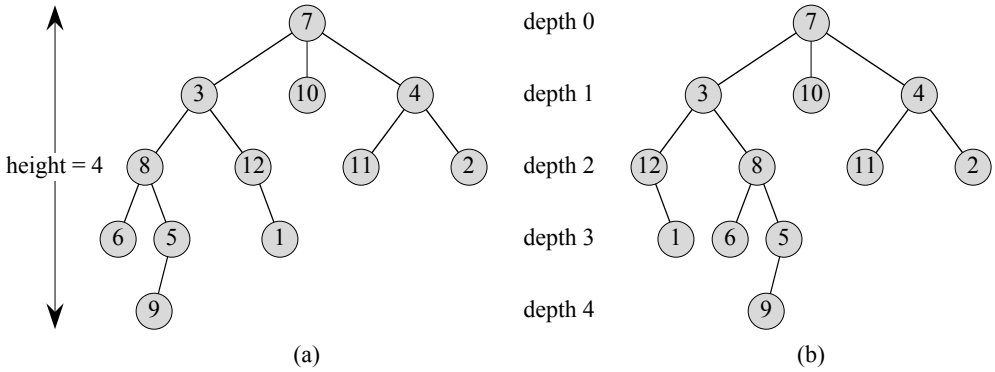

Figure B.6 Rooted and ordered trees. **(a)** A rooted tree with height 4. The tree is drawn in a standard way: the root (node 7) is at the top, its children (nodes with depth 1) are beneath it, their children (nodes with depth 2) are beneath them, and so forth. If the tree is ordered, the relative left-to-right order of the children of a node matters; otherwise it doesn't. **(b)** Another rooted tree. As a rooted tree, it is identical to the tree in (a), but as an ordered tree it is different, since the children of node 3 appear in a different order.

The number of children of a node x in a rooted tree T equals the ***degree*** of x.[6] The length of the simple path from the root r to a node x is the ***depth*** of x in T. A ***level*** of a tree consists of all nodes at the same depth. The ***height*** of a node in a tree is the number of edges on the longest simple downward path from the node to a leaf, and the height of a tree is the height of its root. The height of a tree is also equal to the largest depth of any node in the tree.

An ***ordered tree*** is a rooted tree in which the children of each node are ordered. That is, if a node has k children, then there is a first child, a second child, ..., and a kth child. The two trees in Figure B.6 are different when considered to be ordered trees, but the same when considered to be just rooted trees.

B.5.3 Binary and positional trees

We define binary trees recursively. A ***binary tree*** T is a structure defined on a finite set of nodes that either

- contains no nodes, or

[6] Notice that the degree of a node depends on whether we consider T to be a rooted tree or a free tree. The degree of a vertex in a free tree is, as in any undirected graph, the number of adjacent vertices. In a rooted tree, however, the degree is the number of children—the parent of a node does not count toward its degree.

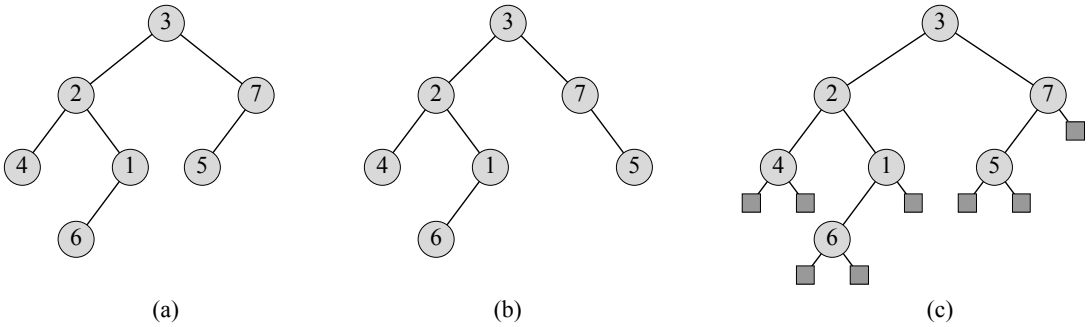

Figure B.7 Binary trees. **(a)** A binary tree drawn in a standard way. The left child of a node is drawn beneath the node and to the left. The right child is drawn beneath and to the right. **(b)** A binary tree different from the one in (a). In (a), the left child of node 7 is 5 and the right child is absent. In (b), the left child of node 7 is absent and the right child is 5. As ordered trees, these trees are the same, but as binary trees, they are distinct. **(c)** The binary tree in (a) represented by the internal nodes of a full binary tree: an ordered tree in which each internal node has degree 2. The leaves in the tree are shown as squares.

- is composed of three disjoint sets of nodes: a ***root*** node, a binary tree called its ***left subtree***, and a binary tree called its ***right subtree***.

The binary tree that contains no nodes is called the ***empty tree*** or ***null tree***, sometimes denoted NIL. If the left subtree is nonempty, its root is called the ***left child*** of the root of the entire tree. Likewise, the root of a nonnull right subtree is the ***right child*** of the root of the entire tree. If a subtree is the null tree NIL, we say that the child is ***absent*** or ***missing***. Figure B.7(a) shows a binary tree.

A binary tree is not simply an ordered tree in which each node has degree at most 2. For example, in a binary tree, if a node has just one child, the position of the child—whether it is the ***left child*** or the ***right child***—matters. In an ordered tree, there is no distinguishing a sole child as being either left or right. Figure B.7(b) shows a binary tree that differs from the tree in Figure B.7(a) because of the position of one node. Considered as ordered trees, however, the two trees are identical.

We can represent the positioning information in a binary tree by the internal nodes of an ordered tree, as shown in Figure B.7(c). The idea is to replace each missing child in the binary tree with a node having no children. These leaf nodes are drawn as squares in the figure. The tree that results is a ***full binary tree***: each node is either a leaf or has degree exactly 2. There are no degree-1 nodes. Consequently, the order of the children of a node preserves the position information.

We can extend the positioning information that distinguishes binary trees from ordered trees to trees with more than 2 children per node. In a ***positional tree***, the

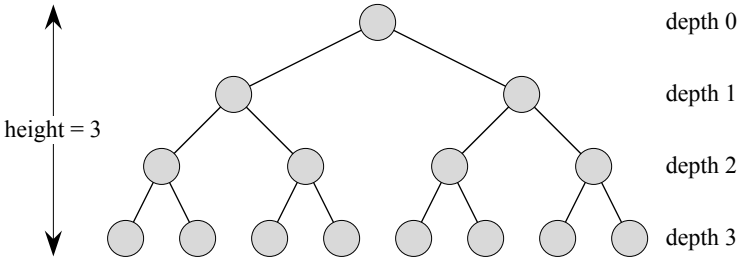

Figure B.8 A complete binary tree of height 3 with 8 leaves and 7 internal nodes.

children of a node are labeled with distinct positive integers. The ith child of a node is ***absent*** if no child is labeled with integer i. A ***k-ary*** tree is a positional tree in which for every node, all children with labels greater than k are missing. Thus, a binary tree is a k-ary tree with $k = 2$.

A ***complete k-ary tree*** is a k-ary tree in which all leaves have the same depth and all internal nodes have degree k. Figure B.8 shows a complete binary tree of height 3. How many leaves does a complete k-ary tree of height h have? The root has k children at depth 1, each of which has k children at depth 2, etc. Thus, the number of leaves at depth h is k^h. Consequently, the height of a complete k-ary tree with n leaves is $\log_k n$. The number of internal nodes of a complete k-ary tree of height h is

$$\begin{aligned} 1 + k + k^2 + \cdots + k^{h-1} &= \sum_{i=0}^{h-1} k^i \\ &= \frac{k^h - 1}{k - 1} \end{aligned}$$

by equation (A.5). Thus, a complete binary tree has $2^h - 1$ internal nodes.

Exercises

B.5-1

Draw all the free trees composed of the three vertices x, y, and z. Draw all the rooted trees with nodes x, y, and z with x as the root. Draw all the ordered trees with nodes x, y, and z with x as the root. Draw all the binary trees with nodes x, y, and z with x as the root.

B.5-2
Let $G = (V, E)$ be a directed acyclic graph in which there is a vertex $v_0 \in V$ such that there exists a unique path from v_0 to every vertex $v \in V$. Prove that the undirected version of G forms a tree.

B.5-3
Show by induction that the number of degree-2 nodes in any nonempty binary tree is 1 fewer than the number of leaves. Conclude that the number of internal nodes in a full binary tree is 1 fewer than the number of leaves.

B.5-4
Use induction to show that a nonempty binary tree with n nodes has height at least $\lfloor \lg n \rfloor$.

B.5-5 ⋆
The ***internal path length*** of a full binary tree is the sum, taken over all internal nodes of the tree, of the depth of each node. Likewise, the ***external path length*** is the sum, taken over all leaves of the tree, of the depth of each leaf. Consider a full binary tree with n internal nodes, internal path length i, and external path length e. Prove that $e = i + 2n$.

B.5-6 ⋆
Let us associate a "weight" $w(x) = 2^{-d}$ with each leaf x of depth d in a binary tree T, and let L be the set of leaves of T. Prove that $\sum_{x \in L} w(x) \leq 1$. (This is known as the ***Kraft inequality***.)

B.5-7 ⋆
Show that if $L \geq 2$, then every binary tree with L leaves contains a subtree having between $L/3$ and $2L/3$ leaves, inclusive.

Problems

B-1 Graph coloring
Given an undirected graph $G = (V, E)$, a ***k-coloring*** of G is a function $c : V \to \{0, 1, \ldots, k-1\}$ such that $c(u) \neq c(v)$ for every edge $(u, v) \in E$. In other words, the numbers $0, 1, \ldots, k-1$ represent the k colors, and adjacent vertices must have different colors.

a. Show that any tree is 2-colorable.

b. Show that the following are equivalent:

1. G is bipartite.
2. G is 2-colorable.
3. G has no cycles of odd length.

c. Let d be the maximum degree of any vertex in a graph G. Prove that we can color G with $d + 1$ colors.

d. Show that if G has $O(|V|)$ edges, then we can color G with $O(\sqrt{|V|})$ colors.

B-2 Friendly graphs

Reword each of the following statements as a theorem about undirected graphs, and then prove it. Assume that friendship is symmetric but not reflexive.

a. Any group of at least two people contains at least two people with the same number of friends in the group.

b. Every group of six people contains either at least three mutual friends or at least three mutual strangers.

c. Any group of people can be partitioned into two subgroups such that at least half the friends of each person belong to the subgroup of which that person is *not* a member.

d. If everyone in a group is the friend of at least half the people in the group, then the group can be seated around a table in such a way that everyone is seated between two friends.

B-3 Bisecting trees

Many divide-and-conquer algorithms that operate on graphs require that the graph be bisected into two nearly equal-sized subgraphs, which are induced by a partition of the vertices. This problem investigates bisections of trees formed by removing a small number of edges. We require that whenever two vertices end up in the same subtree after removing edges, then they must be in the same partition.

a. Show that we can partition the vertices of any n-vertex binary tree into two sets A and B, such that $|A| \leq 3n/4$ and $|B| \leq 3n/4$, by removing a single edge.

b. Show that the constant $3/4$ in part (a) is optimal in the worst case by giving an example of a simple binary tree whose most evenly balanced partition upon removal of a single edge has $|A| = 3n/4$.

c. Show that by removing at most $O(\lg n)$ edges, we can partition the vertices of any n-vertex binary tree into two sets A and B such that $|A| = \lfloor n/2 \rfloor$ and $|B| = \lceil n/2 \rceil$.

Appendix notes

G. Boole pioneered the development of symbolic logic, and he introduced many of the basic set notations in a book published in 1854. Modern set theory was created by G. Cantor during the period 1874–1895. Cantor focused primarily on sets of infinite cardinality. The term "function" is attributed to G. W. Leibniz, who used it to refer to several kinds of mathematical formulas. His limited definition has been generalized many times. Graph theory originated in 1736, when L. Euler proved that it was impossible to cross each of the seven bridges in the city of Königsberg exactly once and return to the starting point.

The book by Harary [160] provides a useful compendium of many definitions and results from graph theory.

C Counting and Probability

This appendix reviews elementary combinatorics and probability theory. If you have a good background in these areas, you may want to skim the beginning of this appendix lightly and concentrate on the later sections. Most of this book's chapters do not require probability, but for some chapters it is essential.

Section C.1 reviews elementary results in counting theory, including standard formulas for counting permutations and combinations. The axioms of probability and basic facts concerning probability distributions form Section C.2. Random variables are introduced in Section C.3, along with the properties of expectation and variance. Section C.4 investigates the geometric and binomial distributions that arise from studying Bernoulli trials. The study of the binomial distribution continues in Section C.5, an advanced discussion of the "tails" of the distribution.

C.1 Counting

Counting theory tries to answer the question "How many?" without actually enumerating all the choices. For example, we might ask, "How many different n-bit numbers are there?" or "How many orderings of n distinct elements are there?" In this section, we review the elements of counting theory. Since some of the material assumes a basic understanding of sets, you might wish to start by reviewing the material in Section B.1.

Rules of sum and product

We can sometimes express a set of items that we wish to count as a union of disjoint sets or as a Cartesian product of sets.

The ***rule of sum*** says that the number of ways to choose one element from one of two *disjoint* sets is the sum of the cardinalities of the sets. That is, if A and B are two finite sets with no members in common, then $|A \cup B| = |A| + |B|$, which

follows from equation (B.3). For example, each position on a car's license plate is a letter or a digit. The number of possibilities for each position is therefore $26 + 10 = 36$, since there are 26 choices if it is a letter and 10 choices if it is a digit.

The ***rule of product*** says that the number of ways to choose an ordered pair is the number of ways to choose the first element times the number of ways to choose the second element. That is, if A and B are two finite sets, then $|A \times B| = |A| \cdot |B|$, which is simply equation (B.4). For example, if an ice-cream parlor offers 28 flavors of ice cream and 4 toppings, the number of possible sundaes with one scoop of ice cream and one topping is $28 \cdot 4 = 112$.

Strings

A ***string*** over a finite set S is a sequence of elements of S. For example, there are 8 binary strings of length 3:

$$000, 001, 010, 011, 100, 101, 110, 111 .$$

We sometimes call a string of length k a ***k-string***. A ***substring*** s' of a string s is an ordered sequence of consecutive elements of s. A ***k-substring*** of a string is a substring of length k. For example, 010 is a 3-substring of 01101001 (the 3-substring that begins in position 4), but 111 is not a substring of 01101001.

We can view a k-string over a set S as an element of the Cartesian product S^k of k-tuples; thus, there are $|S|^k$ strings of length k. For example, the number of binary k-strings is 2^k. Intuitively, to construct a k-string over an n-set, we have n ways to pick the first element; for each of these choices, we have n ways to pick the second element; and so forth k times. This construction leads to the k-fold product $n \cdot n \cdots n = n^k$ as the number of k-strings.

Permutations

A ***permutation*** of a finite set S is an ordered sequence of all the elements of S, with each element appearing exactly once. For example, if $S = \{a, b, c\}$, then S has 6 permutations:

$$abc, acb, bac, bca, cab, cba .$$

There are $n!$ permutations of a set of n elements, since we can choose the first element of the sequence in n ways, the second in $n - 1$ ways, the third in $n - 2$ ways, and so on.

A ***k-permutation*** of S is an ordered sequence of k elements of S, with no element appearing more than once in the sequence. (Thus, an ordinary permutation is an n-permutation of an n-set.) The twelve 2-permutations of the set $\{a, b, c, d\}$ are

$ab, ac, ad, ba, bc, bd, ca, cb, cd, da, db, dc$.

The number of k-permutations of an n-set is

$$n(n-1)(n-2)\cdots(n-k+1) = \frac{n!}{(n-k)!}\,, \tag{C.1}$$

since we have n ways to choose the first element, $n-1$ ways to choose the second element, and so on, until we have selected k elements, the last being a selection from the remaining $n-k+1$ elements.

Combinations

A ***k*-combination** of an n-set S is simply a k-subset of S. For example, the 4-set $\{a, b, c, d\}$ has six 2-combinations:

ab, ac, ad, bc, bd, cd .

(Here we use the shorthand of denoting the 2-subset $\{a, b\}$ by ab, and so on.) We can construct a k-combination of an n-set by choosing k distinct (different) elements from the n-set. The order in which we select the elements does not matter.

We can express the number of k-combinations of an n-set in terms of the number of k-permutations of an n-set. Every k-combination has exactly $k!$ permutations of its elements, each of which is a distinct k-permutation of the n-set. Thus, the number of k-combinations of an n-set is the number of k-permutations divided by $k!$; from equation (C.1), this quantity is

$$\frac{n!}{k!\,(n-k)!}\,. \tag{C.2}$$

For $k = 0$, this formula tells us that the number of ways to choose 0 elements from an n-set is 1 (not 0), since $0! = 1$.

Binomial coefficients

The notation $\binom{n}{k}$ (read "n choose k") denotes the number of k-combinations of an n-set. From equation (C.2), we have

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

This formula is symmetric in k and $n-k$:

$$\binom{n}{k} = \binom{n}{n-k}\,. \tag{C.3}$$

These numbers are also known as ***binomial coefficients***, due to their appearance in the ***binomial expansion***:

$$(x+y)^n = \sum_{k=0}^{n} \binom{n}{k} x^k y^{n-k} . \tag{C.4}$$

A special case of the binomial expansion occurs when $x = y = 1$:

$$2^n = \sum_{k=0}^{n} \binom{n}{k} .$$

This formula corresponds to counting the 2^n binary n-strings by the number of 1s they contain: $\binom{n}{k}$ binary n-strings contain exactly k 1s, since we have $\binom{n}{k}$ ways to choose k out of the n positions in which to place the 1s.

Many identities involve binomial coefficients. The exercises at the end of this section give you the opportunity to prove a few.

Binomial bounds

We sometimes need to bound the size of a binomial coefficient. For $1 \le k \le n$, we have the lower bound

$$\begin{aligned}
\binom{n}{k} &= \frac{n(n-1)\cdots(n-k+1)}{k(k-1)\cdots 1} \\
&= \left(\frac{n}{k}\right)\left(\frac{n-1}{k-1}\right)\cdots\left(\frac{n-k+1}{1}\right) \\
&\ge \left(\frac{n}{k}\right)^k .
\end{aligned}$$

Taking advantage of the inequality $k! \ge (k/e)^k$ derived from Stirling's approximation (3.18), we obtain the upper bounds

$$\begin{aligned}
\binom{n}{k} &= \frac{n(n-1)\cdots(n-k+1)}{k(k-1)\cdots 1} \\
&\le \frac{n^k}{k!} \\
&\le \left(\frac{en}{k}\right)^k . \qquad \text{(C.5)}
\end{aligned}$$

For all integers k such that $0 \le k \le n$, we can use induction (see Exercise C.1-12) to prove the bound

$$\binom{n}{k} \leq \frac{n^n}{k^k (n-k)^{n-k}} , \tag{C.6}$$

where for convenience we assume that $0^0 = 1$. For $k = \lambda n$, where $0 \leq \lambda \leq 1$, we can rewrite this bound as

$$\begin{aligned} \binom{n}{\lambda n} &\leq \frac{n^n}{(\lambda n)^{\lambda n} ((1-\lambda)n)^{(1-\lambda)n}} \\ &= \left(\left(\frac{1}{\lambda}\right)^{\lambda} \left(\frac{1}{1-\lambda}\right)^{1-\lambda} \right)^n \\ &= 2^{n\,H(\lambda)} , \end{aligned}$$

where

$$H(\lambda) = -\lambda \lg \lambda - (1-\lambda) \lg(1-\lambda) \tag{C.7}$$

is the ***(binary) entropy function*** and where, for convenience, we assume that $0 \lg 0 = 0$, so that $H(0) = H(1) = 0$.

Exercises

C.1-1

How many k-substrings does an n-string have? (Consider identical k-substrings at different positions to be different.) How many substrings does an n-string have in total?

C.1-2

An n-input, m-output ***boolean function*** is a function from $\{\text{TRUE}, \text{FALSE}\}^n$ to $\{\text{TRUE}, \text{FALSE}\}^m$. How many n-input, 1-output boolean functions are there? How many n-input, m-output boolean functions are there?

C.1-3

In how many ways can n professors sit around a circular conference table? Consider two seatings to be the same if one can be rotated to form the other.

C.1-4

In how many ways can we choose three distinct numbers from the set $\{1, 2, \ldots, 99\}$ so that their sum is even?

C.1-5
Prove the identity

$$\binom{n}{k} = \frac{n}{k}\binom{n-1}{k-1} \tag{C.8}$$

for $0 < k \leq n$.

C.1-6
Prove the identity

$$\binom{n}{k} = \frac{n}{n-k}\binom{n-1}{k}$$

for $0 \leq k < n$.

C.1-7
To choose k objects from n, you can make one of the objects distinguished and consider whether the distinguished object is chosen. Use this approach to prove that

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

C.1-8
Using the result of Exercise C.1-7, make a table for $n = 0, 1, \ldots, 6$ and $0 \leq k \leq n$ of the binomial coefficients $\binom{n}{k}$ with $\binom{0}{0}$ at the top, $\binom{1}{0}$ and $\binom{1}{1}$ on the next line, and so forth. Such a table of binomial coefficients is called ***Pascal's triangle***.

C.1-9
Prove that

$$\sum_{i=1}^{n} i = \binom{n+1}{2}.$$

C.1-10
Show that for any integers $n \geq 0$ and $0 \leq k \leq n$, the expression $\binom{n}{k}$ achieves its maximum value when $k = \lfloor n/2 \rfloor$ or $k = \lceil n/2 \rceil$.

C.1-11 ⋆
Argue that for any integers $n \geq 0$, $j \geq 0$, $k \geq 0$, and $j + k \leq n$,

$$\binom{n}{j+k} \leq \binom{n}{j}\binom{n-j}{k}. \tag{C.9}$$

Provide both an algebraic proof and an argument based on a method for choosing $j + k$ items out of n. Give an example in which equality does not hold.

C.1-12 ⋆
Use induction on all integers k such that $0 \le k \le n/2$ to prove inequality (C.6), and use equation (C.3) to extend it to all integers k such that $0 \le k \le n$.

C.1-13 ⋆
Use Stirling's approximation to prove that

$$\binom{2n}{n} = \frac{2^{2n}}{\sqrt{\pi n}}(1 + O(1/n)) \; . \tag{C.10}$$

C.1-14 ⋆
By differentiating the entropy function $H(\lambda)$, show that it achieves its maximum value at $\lambda = 1/2$. What is $H(1/2)$?

C.1-15 ⋆
Show that for any integer $n \ge 0$,

$$\sum_{k=0}^{n} \binom{n}{k} k = n2^{n-1} \; . \tag{C.11}$$

C.2 Probability

Probability is an essential tool for the design and analysis of probabilistic and randomized algorithms. This section reviews basic probability theory.

We define probability in terms of a ***sample space*** S, which is a set whose elements are called ***elementary events***. We can think of each elementary event as a possible outcome of an experiment. For the experiment of flipping two distinguishable coins, with each individual flip resulting in a head (H) or a tail (T), we can view the sample space as consisting of the set of all possible 2-strings over $\{\text{H}, \text{T}\}$:

$$S = \{\text{HH}, \text{HT}, \text{TH}, \text{TT}\} \; .$$

An ***event*** is a subset[1] of the sample space S. For example, in the experiment of flipping two coins, the event of obtaining one head and one tail is $\{\text{HT}, \text{TH}\}$. The event S is called the ***certain event***, and the event $\emptyset$ is called the ***null event***. We say that two events A and B are ***mutually exclusive*** if $A \cap B = \emptyset$. We sometimes treat an elementary event $s \in S$ as the event $\{s\}$. By definition, all elementary events are mutually exclusive.

Axioms of probability

A ***probability distribution*** $\Pr\{\}$ on a sample space S is a mapping from events of S to real numbers satisfying the following ***probability axioms***:

1. $\Pr\{A\} \geq 0$ for any event A.
2. $\Pr\{S\} = 1$.
3. $\Pr\{A \cup B\} = \Pr\{A\} + \Pr\{B\}$ for any two mutually exclusive events A and B. More generally, for any (finite or countably infinite) sequence of events $A_1, A_2, \ldots$ that are pairwise mutually exclusive,

$$\Pr\left\{\bigcup_i A_i\right\} = \sum_i \Pr\{A_i\} \ .$$

We call $\Pr\{A\}$ the ***probability*** of the event A. We note here that axiom 2 is a normalization requirement: there is really nothing fundamental about choosing 1 as the probability of the certain event, except that it is natural and convenient.

Several results follow immediately from these axioms and basic set theory (see Section B.1). The null event $\emptyset$ has probability $\Pr\{\emptyset\} = 0$. If $A \subseteq B$, then $\Pr\{A\} \leq \Pr\{B\}$. Using $\overline{A}$ to denote the event $S - A$ (the ***complement*** of A), we have $\Pr\{\overline{A}\} = 1 - \Pr\{A\}$. For any two events A and B,

$$\Pr\{A \cup B\} = \Pr\{A\} + \Pr\{B\} - \Pr\{A \cap B\} \tag{C.12}$$

$$\leq \Pr\{A\} + \Pr\{B\} \ . \tag{C.13}$$

---

[1] For a general probability distribution, there may be some subsets of the sample space S that are not considered to be events. This situation usually arises when the sample space is uncountably infinite. The main requirement for what subsets are events is that the set of events of a sample space be closed under the operations of taking the complement of an event, forming the union of a finite or countable number of events, and taking the intersection of a finite or countable number of events. Most of the probability distributions we shall see are over finite or countable sample spaces, and we shall generally consider all subsets of a sample space to be events. A notable exception is the continuous uniform probability distribution, which we shall see shortly.

In our coin-flipping example, suppose that each of the four elementary events has probability $1/4$. Then the probability of getting at least one head is

$$\begin{aligned}\Pr\{\text{HH}, \text{HT}, \text{TH}\} &= \Pr\{\text{HH}\} + \Pr\{\text{HT}\} + \Pr\{\text{TH}\} \\ &= 3/4 .\end{aligned}$$

Alternatively, since the probability of getting strictly less than one head is $\Pr\{\text{TT}\} = 1/4$, the probability of getting at least one head is $1 - 1/4 = 3/4$.

Discrete probability distributions

A probability distribution is ***discrete*** if it is defined over a finite or countably infinite sample space. Let S be the sample space. Then for any event A,

$$\Pr\{A\} = \sum_{s \in A} \Pr\{s\} ,$$

since elementary events, specifically those in A, are mutually exclusive. If S is finite and every elementary event $s \in S$ has probability

$$\Pr\{s\} = 1/|S| ,$$

then we have the ***uniform probability distribution*** on S. In such a case the experiment is often described as "picking an element of S at random."

As an example, consider the process of flipping a ***fair coin***, one for which the probability of obtaining a head is the same as the probability of obtaining a tail, that is, $1/2$. If we flip the coin n times, we have the uniform probability distribution defined on the sample space $S = \{\text{H}, \text{T}\}^n$, a set of size 2^n. We can represent each elementary event in S as a string of length n over $\{\text{H}, \text{T}\}$, each string occurring with probability $1/2^n$. The event

$$A = \{\text{exactly } k \text{ heads and exactly } n - k \text{ tails occur}\}$$

is a subset of S of size $|A| = \binom{n}{k}$, since $\binom{n}{k}$ strings of length n over $\{\text{H}, \text{T}\}$ contain exactly k H's. The probability of event A is thus $\Pr\{A\} = \binom{n}{k}/2^n$.

Continuous uniform probability distribution

The continuous uniform probability distribution is an example of a probability distribution in which not all subsets of the sample space are considered to be events. The continuous uniform probability distribution is defined over a closed interval $[a, b]$ of the reals, where $a < b$. Our intuition is that each point in the interval $[a, b]$ should be "equally likely." There are an uncountable number of points, however, so if we give all points the same finite, positive probability, we cannot simultaneously satisfy axioms 2 and 3. For this reason, we would like to associate a

probability only with *some* of the subsets of S, in such a way that the axioms are satisfied for these events.

For any closed interval $[c, d]$, where $a \le c \le d \le b$, the ***continuous uniform probability distribution*** defines the probability of the event $[c, d]$ to be

$$\Pr\{[c, d]\} = \frac{d - c}{b - a} .$$

Note that for any point $x = [x, x]$, the probability of x is 0. If we remove the endpoints of an interval $[c, d]$, we obtain the open interval (c, d). Since $[c, d] = [c, c] \cup (c, d) \cup [d, d]$, axiom 3 gives us $\Pr\{[c, d]\} = \Pr\{(c, d)\}$. Generally, the set of events for the continuous uniform probability distribution contains any subset of the sample space $[a, b]$ that can be obtained by a finite or countable union of open and closed intervals, as well as certain more complicated sets.

Conditional probability and independence

Sometimes we have some prior partial knowledge about the outcome of an experiment. For example, suppose that a friend has flipped two fair coins and has told you that at least one of the coins showed a head. What is the probability that both coins are heads? The information given eliminates the possibility of two tails. The three remaining elementary events are equally likely, so we infer that each occurs with probability $1/3$. Since only one of these elementary events shows two heads, the answer to our question is $1/3$.

Conditional probability formalizes the notion of having prior partial knowledge of the outcome of an experiment. The ***conditional probability*** of an event A given that another event B occurs is defined to be

$$\Pr\{A \mid B\} = \frac{\Pr\{A \cap B\}}{\Pr\{B\}} \tag{C.14}$$

whenever $\Pr\{B\} \neq 0$. (We read "$\Pr\{A \mid B\}$" as "the probability of A given B.") Intuitively, since we are given that event B occurs, the event that A also occurs is $A \cap B$. That is, $A \cap B$ is the set of outcomes in which both A and B occur. Because the outcome is one of the elementary events in B, we normalize the probabilities of all the elementary events in B by dividing them by $\Pr\{B\}$, so that they sum to 1. The conditional probability of A given B is, therefore, the ratio of the probability of event $A \cap B$ to the probability of event B. In the example above, A is the event that both coins are heads, and B is the event that at least one coin is a head. Thus, $\Pr\{A \mid B\} = (1/4)/(3/4) = 1/3$.

Two events are ***independent*** if

$$\Pr\{A \cap B\} = \Pr\{A\} \Pr\{B\} , \tag{C.15}$$

which is equivalent, if $\Pr\{B\} \neq 0$, to the condition

$$\Pr\{A \mid B\} = \Pr\{A\} .$$

For example, suppose that we flip two fair coins and that the outcomes are independent. Then the probability of two heads is $(1/2)(1/2) = 1/4$. Now suppose that one event is that the first coin comes up heads and the other event is that the coins come up differently. Each of these events occurs with probability $1/2$, and the probability that both events occur is $1/4$; thus, according to the definition of independence, the events are independent—even though you might think that both events depend on the first coin. Finally, suppose that the coins are welded together so that they both fall heads or both fall tails and that the two possibilities are equally likely. Then the probability that each coin comes up heads is $1/2$, but the probability that they both come up heads is $1/2 \neq (1/2)(1/2)$. Consequently, the event that one comes up heads and the event that the other comes up heads are not independent.

A collection $A_1, A_2, \ldots, A_n$ of events is said to be ***pairwise independent*** if

$$\Pr\{A_i \cap A_j\} = \Pr\{A_i\}\Pr\{A_j\}$$

for all $1 \leq i < j \leq n$. We say that the events of the collection are ***(mutually) independent*** if every k-subset $A_{i_1}, A_{i_2}, \ldots, A_{i_k}$ of the collection, where $2 \leq k \leq n$ and $1 \leq i_1 < i_2 < \cdots < i_k \leq n$, satisfies

$$\Pr\{A_{i_1} \cap A_{i_2} \cap \cdots \cap A_{i_k}\} = \Pr\{A_{i_1}\}\Pr\{A_{i_2}\}\cdots\Pr\{A_{i_k}\} .$$

For example, suppose we flip two fair coins. Let A_1 be the event that the first coin is heads, let A_2 be the event that the second coin is heads, and let A_3 be the event that the two coins are different. We have

$$\begin{aligned}
\Pr\{A_1\} &= 1/2 , \\
\Pr\{A_2\} &= 1/2 , \\
\Pr\{A_3\} &= 1/2 , \\
\Pr\{A_1 \cap A_2\} &= 1/4 , \\
\Pr\{A_1 \cap A_3\} &= 1/4 , \\
\Pr\{A_2 \cap A_3\} &= 1/4 , \\
\Pr\{A_1 \cap A_2 \cap A_3\} &= 0 .
\end{aligned}$$

Since for $1 \leq i < j \leq 3$, we have $\Pr\{A_i \cap A_j\} = \Pr\{A_i\}\Pr\{A_j\} = 1/4$, the events A_1, A_2, and A_3 are pairwise independent. The events are not mutually independent, however, because $\Pr\{A_1 \cap A_2 \cap A_3\} = 0$ and $\Pr\{A_1\}\Pr\{A_2\}\Pr\{A_3\} = 1/8 \neq 0$.

Bayes's theorem

From the definition of conditional probability (C.14) and the commutative law $A \cap B = B \cap A$, it follows that for two events A and B, each with nonzero probability,

$$\begin{aligned} \Pr\{A \cap B\} &= \Pr\{B\} \Pr\{A \mid B\} \\ &= \Pr\{A\} \Pr\{B \mid A\} . \end{aligned} \tag{C.16}$$

Solving for $\Pr\{A \mid B\}$, we obtain

$$\Pr\{A \mid B\} = \frac{\Pr\{A\} \Pr\{B \mid A\}}{\Pr\{B\}} , \tag{C.17}$$

which is known as ***Bayes's theorem***. The denominator $\Pr\{B\}$ is a normalizing constant, which we can reformulate as follows. Since $B = (B \cap A) \cup (B \cap \overline{A})$, and since $B \cap A$ and $B \cap \overline{A}$ are mutually exclusive events,

$$\begin{aligned} \Pr\{B\} &= \Pr\{B \cap A\} + \Pr\left\{B \cap \overline{A}\right\} \\ &= \Pr\{A\} \Pr\{B \mid A\} + \Pr\left\{\overline{A}\right\} \Pr\left\{B \mid \overline{A}\right\} . \end{aligned}$$

Substituting into equation (C.17), we obtain an equivalent form of Bayes's theorem:

$$\Pr\{A \mid B\} = \frac{\Pr\{A\} \Pr\{B \mid A\}}{\Pr\{A\} \Pr\{B \mid A\} + \Pr\left\{\overline{A}\right\} \Pr\left\{B \mid \overline{A}\right\}} . \tag{C.18}$$

Bayes's theorem can simplify the computing of conditional probabilities. For example, suppose that we have a fair coin and a biased coin that always comes up heads. We run an experiment consisting of three independent events: we choose one of the two coins at random, we flip that coin once, and then we flip it again. Suppose that the coin we have chosen comes up heads both times. What is the probability that it is biased?

We solve this problem using Bayes's theorem. Let A be the event that we choose the biased coin, and let B be the event that the chosen coin comes up heads both times. We wish to determine $\Pr\{A \mid B\}$. We have $\Pr\{A\} = 1/2$, $\Pr\{B \mid A\} = 1$, $\Pr\left\{\overline{A}\right\} = 1/2$, and $\Pr\left\{B \mid \overline{A}\right\} = 1/4$; hence,

$$\begin{aligned} \Pr\{A \mid B\} &= \frac{(1/2) \cdot 1}{(1/2) \cdot 1 + (1/2) \cdot (1/4)} \\ &= 4/5 . \end{aligned}$$

Exercises

C.2-1

Professor Rosencrantz flips a fair coin once. Professor Guildenstern flips a fair coin twice. What is the probability that Professor Rosencrantz obtains more heads than Professor Guildenstern?

C.2-2
Prove ***Boole's inequality***: For any finite or countably infinite sequence of events $A_1, A_2, \ldots$,

$$\Pr\{A_1 \cup A_2 \cup \cdots\} \leq \Pr\{A_1\} + \Pr\{A_2\} + \cdots . \tag{C.19}$$

C.2-3
Suppose we shuffle a deck of 10 cards, each bearing a distinct number from 1 to 10, to mix the cards thoroughly. We then remove three cards, one at a time, from the deck. What is the probability that we select the three cards in sorted (increasing) order?

C.2-4
Prove that

$$\Pr\{A \mid B\} + \Pr\left\{\overline{A} \mid B\right\} = 1 .$$

C.2-5
Prove that for any collection of events $A_1, A_2, \ldots, A_n$,

$$\begin{aligned}\Pr\{A_1 \cap A_2 \cap \cdots \cap A_n\} = \Pr\{A_1\} \cdot \Pr\{A_2 \mid A_1\} \cdot \Pr\{A_3 \mid A_1 \cap A_2\} \cdots \\ \Pr\{A_n \mid A_1 \cap A_2 \cap \cdots \cap A_{n-1}\} .\end{aligned}$$

C.2-6 ⋆
Describe a procedure that takes as input two integers a and b such that $0 < a < b$ and, using fair coin flips, produces as output heads with probability a/b and tails with probability $(b - a)/b$. Give a bound on the expected number of coin flips, which should be $O(1)$. (*Hint:* Represent a/b in binary.)

C.2-7 ⋆
Show how to construct a set of n events that are pairwise independent but such that no subset of $k > 2$ of them is mutually independent.

C.2-8 ⋆
Two events A and B are ***conditionally independent***, given C, if

$$\Pr\{A \cap B \mid C\} = \Pr\{A \mid C\} \cdot \Pr\{B \mid C\} .$$

Give a simple but nontrivial example of two events that are not independent but are conditionally independent given a third event.

C.2-9 ⋆
You are a contestant in a game show in which a prize is hidden behind one of three curtains. You will win the prize if you select the correct curtain. After you

have picked one curtain but before the curtain is lifted, the emcee lifts one of the other curtains, knowing that it will reveal an empty stage, and asks if you would like to switch from your current selection to the remaining curtain. How would your chances change if you switch? (This question is the celebrated ***Monty Hall problem***, named after a game-show host who often presented contestants with just this dilemma.)

C.2-10 ⋆

A prison warden has randomly picked one prisoner among three to go free. The other two will be executed. The guard knows which one will go free but is forbidden to give any prisoner information regarding his status. Let us call the prisoners X, Y, and Z. Prisoner X asks the guard privately which of Y or Z will be executed, arguing that since he already knows that at least one of them must die, the guard won't be revealing any information about his own status. The guard tells X that Y is to be executed. Prisoner X feels happier now, since he figures that either he or prisoner Z will go free, which means that his probability of going free is now $1/2$. Is he right, or are his chances still $1/3$? Explain.

C.3 Discrete random variables

A ***(discrete) random variable*** X is a function from a finite or countably infinite sample space S to the real numbers. It associates a real number with each possible outcome of an experiment, which allows us to work with the probability distribution induced on the resulting set of numbers. Random variables can also be defined for uncountably infinite sample spaces, but they raise technical issues that are unnecessary to address for our purposes. Henceforth, we shall assume that random variables are discrete.

For a random variable X and a real number x, we define the event $X = x$ to be $\{s \in S : X(s) = x\}$; thus,

$$\Pr\{X = x\} = \sum_{s \in S : X(s) = x} \Pr\{s\} \ .$$

The function

$$f(x) = \Pr\{X = x\}$$

is the ***probability density function*** of the random variable X. From the probability axioms, $\Pr\{X = x\} \geq 0$ and $\sum_x \Pr\{X = x\} = 1$.

As an example, consider the experiment of rolling a pair of ordinary, 6-sided dice. There are 36 possible elementary events in the sample space. We assume

that the probability distribution is uniform, so that each elementary event $s \in S$ is equally likely: $\Pr\{s\} = 1/36$. Define the random variable X to be the *maximum* of the two values showing on the dice. We have $\Pr\{X = 3\} = 5/36$, since X assigns a value of 3 to 5 of the 36 possible elementary events, namely, $(1, 3)$, $(2, 3)$, $(3, 3)$, $(3, 2)$, and $(3, 1)$.

We often define several random variables on the same sample space. If X and Y are random variables, the function

$$f(x, y) = \Pr\{X = x \text{ and } Y = y\}$$

is the ***joint probability density function*** of X and Y. For a fixed value y,

$$\Pr\{Y = y\} = \sum_x \Pr\{X = x \text{ and } Y = y\} ,$$

and similarly, for a fixed value x,

$$\Pr\{X = x\} = \sum_y \Pr\{X = x \text{ and } Y = y\} .$$

Using the definition (C.14) of conditional probability, we have

$$\Pr\{X = x \mid Y = y\} = \frac{\Pr\{X = x \text{ and } Y = y\}}{\Pr\{Y = y\}} .$$

We define two random variables X and Y to be ***independent*** if for all x and y, the events $X = x$ and $Y = y$ are independent or, equivalently, if for all x and y, we have $\Pr\{X = x \text{ and } Y = y\} = \Pr\{X = x\} \Pr\{Y = y\}$.

Given a set of random variables defined over the same sample space, we can define new random variables as sums, products, or other functions of the original variables.

Expected value of a random variable

The simplest and most useful summary of the distribution of a random variable is the "average" of the values it takes on. The ***expected value*** (or, synonymously, ***expectation*** or ***mean***) of a discrete random variable X is

$$\mathrm{E}[X] = \sum_x x \cdot \Pr\{X = x\} , \tag{C.20}$$

which is well defined if the sum is finite or converges absolutely. Sometimes the expectation of X is denoted by μ_X or, when the random variable is apparent from context, simply by μ.

Consider a game in which you flip two fair coins. You earn \$3 for each head but lose \$2 for each tail. The expected value of the random variable X representing

your earnings is

$$\begin{aligned}\mathrm{E}[X] &= 6 \cdot \Pr\{2 \text{ H's}\} + 1 \cdot \Pr\{1 \text{ H}, 1 \text{ T}\} - 4 \cdot \Pr\{2 \text{ T's}\} \\ &= 6(1/4) + 1(1/2) - 4(1/4) \\ &= 1 \ .\end{aligned}$$

The expectation of the sum of two random variables is the sum of their expectations, that is,

$$\mathrm{E}[X + Y] = \mathrm{E}[X] + \mathrm{E}[Y] \ , \tag{C.21}$$

whenever $\mathrm{E}[X]$ and $\mathrm{E}[Y]$ are defined. We call this property ***linearity of expectation***, and it holds even if X and Y are not independent. It also extends to finite and absolutely convergent summations of expectations. Linearity of expectation is the key property that enables us to perform probabilistic analyses by using indicator random variables (see Section 5.2).

If X is any random variable, any function $g(x)$ defines a new random variable $g(X)$. If the expectation of $g(X)$ is defined, then

$$\mathrm{E}[g(X)] = \sum_x g(x) \cdot \Pr\{X = x\} \ .$$

Letting $g(x) = ax$, we have for any constant a,

$$\mathrm{E}[aX] = a\mathrm{E}[X] \ . \tag{C.22}$$

Consequently, expectations are linear: for any two random variables X and Y and any constant a,

$$\mathrm{E}[aX + Y] = a\mathrm{E}[X] + \mathrm{E}[Y] \ . \tag{C.23}$$

When two random variables X and Y are independent and each has a defined expectation,

$$\begin{aligned}\mathrm{E}[XY] &= \sum_x \sum_y xy \cdot \Pr\{X = x \text{ and } Y = y\} \\ &= \sum_x \sum_y xy \cdot \Pr\{X = x\} \Pr\{Y = y\} \\ &= \left(\sum_x x \cdot \Pr\{X = x\}\right)\left(\sum_y y \cdot \Pr\{Y = y\}\right) \\ &= \mathrm{E}[X]\,\mathrm{E}[Y] \ .\end{aligned}$$

In general, when n random variables $X_1, X_2, \ldots, X_n$ are mutually independent,

$$\mathrm{E}[X_1 X_2 \cdots X_n] = \mathrm{E}[X_1]\,\mathrm{E}[X_2] \cdots \mathrm{E}[X_n] \ . \tag{C.24}$$

When a random variable X takes on values from the set of natural numbers $\mathbb{N} = \{0, 1, 2, \ldots\}$, we have a nice formula for its expectation:

$$\begin{aligned} \mathrm{E}[X] &= \sum_{i=0}^{\infty} i \cdot \Pr\{X = i\} \\ &= \sum_{i=0}^{\infty} i(\Pr\{X \geq i\} - \Pr\{X \geq i+1\}) \\ &= \sum_{i=1}^{\infty} \Pr\{X \geq i\} \ , \end{aligned} \tag{C.25}$$

since each term $\Pr\{X \geq i\}$ is added in i times and subtracted out $i - 1$ times (except $\Pr\{X \geq 0\}$, which is added in 0 times and not subtracted out at all).

When we apply a convex function $f(x)$ to a random variable X, ***Jensen's inequality*** gives us

$$\mathrm{E}[f(X)] \geq f(\mathrm{E}[X]) \ , \tag{C.26}$$

provided that the expectations exist and are finite. (A function $f(x)$ is ***convex*** if for all x and y and for all $0 \leq \lambda \leq 1$, we have $f(\lambda x + (1-\lambda)y) \leq \lambda f(x) + (1-\lambda) f(y)$.)

Variance and standard deviation

The expected value of a random variable does not tell us how "spread out" the variable's values are. For example, if we have random variables X and Y for which $\Pr\{X = 1/4\} = \Pr\{X = 3/4\} = 1/2$ and $\Pr\{Y = 0\} = \Pr\{Y = 1\} = 1/2$, then both $\mathrm{E}[X]$ and $\mathrm{E}[Y]$ are $1/2$, yet the actual values taken on by Y are farther from the mean than the actual values taken on by X.

The notion of variance mathematically expresses how far from the mean a random variable's values are likely to be. The ***variance*** of a random variable X with mean $\mathrm{E}[X]$ is

$$\begin{aligned} \mathrm{Var}[X] &= \mathrm{E}\left[(X - \mathrm{E}[X])^2\right] \\ &= \mathrm{E}\left[X^2 - 2X\mathrm{E}[X] + \mathrm{E}^2[X]\right] \\ &= \mathrm{E}\left[X^2\right] - 2\mathrm{E}[X\mathrm{E}[X]] + \mathrm{E}^2[X] \\ &= \mathrm{E}\left[X^2\right] - 2\mathrm{E}^2[X] + \mathrm{E}^2[X] \\ &= \mathrm{E}\left[X^2\right] - \mathrm{E}^2[X] \ . \end{aligned} \tag{C.27}$$

To justify the equality $\mathrm{E}[\mathrm{E}^2[X]] = \mathrm{E}^2[X]$, note that because $\mathrm{E}[X]$ is a real number and not a random variable, so is $\mathrm{E}^2[X]$. The equality $\mathrm{E}[X\mathrm{E}[X]] = \mathrm{E}^2[X]$

follows from equation (C.22), with $a = \mathrm{E}[X]$. Rewriting equation (C.27) yields an expression for the expectation of the square of a random variable:

$$\mathrm{E}\left[X^2\right] = \mathrm{Var}[X] + \mathrm{E}^2[X] \ . \tag{C.28}$$

The variance of a random variable X and the variance of aX are related (see Exercise C.3-10):

$$\mathrm{Var}[aX] = a^2\mathrm{Var}[X] \ .$$

When X and Y are independent random variables,

$$\mathrm{Var}[X + Y] = \mathrm{Var}[X] + \mathrm{Var}[Y] \ .$$

In general, if n random variables $X_1, X_2, \ldots, X_n$ are pairwise independent, then

$$\mathrm{Var}\left[\sum_{i=1}^{n} X_i\right] = \sum_{i=1}^{n} \mathrm{Var}[X_i] \ . \tag{C.29}$$

The ***standard deviation*** of a random variable X is the nonnegative square root of the variance of X. The standard deviation of a random variable X is sometimes denoted σ_X or simply σ when the random variable X is understood from context. With this notation, the variance of X is denoted σ^2.

Exercises

C.3-1

Suppose we roll two ordinary, 6-sided dice. What is the expectation of the sum of the two values showing? What is the expectation of the maximum of the two values showing?

C.3-2

An array $A[1\,..\,n]$ contains n distinct numbers that are randomly ordered, with each permutation of the n numbers being equally likely. What is the expectation of the index of the maximum element in the array? What is the expectation of the index of the minimum element in the array?

C.3-3

A carnival game consists of three dice in a cage. A player can bet a dollar on any of the numbers 1 through 6. The cage is shaken, and the payoff is as follows. If the player's number doesn't appear on any of the dice, he loses his dollar. Otherwise, if his number appears on exactly k of the three dice, for $k = 1, 2, 3$, he keeps his dollar and wins k more dollars. What is his expected gain from playing the carnival game once?

C.3-4
Argue that if X and Y are nonnegative random variables, then

$$\mathrm{E}[\max(X, Y)] \leq \mathrm{E}[X] + \mathrm{E}[Y] .$$

C.3-5 ⋆
Let X and Y be independent random variables. Prove that $f(X)$ and $g(Y)$ are independent for any choice of functions f and g.

C.3-6 ⋆
Let X be a nonnegative random variable, and suppose that $\mathrm{E}[X]$ is well defined. Prove ***Markov's inequality***:

$$\Pr\{X \geq t\} \leq \mathrm{E}[X]/t \tag{C.30}$$

for all $t > 0$.

C.3-7 ⋆
Let S be a sample space, and let X and X' be random variables such that $X(s) \geq X'(s)$ for all $s \in S$. Prove that for any real constant t,

$$\Pr\{X \geq t\} \geq \Pr\{X' \geq t\} .$$

C.3-8
Which is larger: the expectation of the square of a random variable, or the square of its expectation?

C.3-9
Show that for any random variable X that takes on only the values 0 and 1, we have $\mathrm{Var}[X] = \mathrm{E}[X]\,\mathrm{E}[1 - X]$.

C.3-10
Prove that $\mathrm{Var}[aX] = a^2\mathrm{Var}[X]$ from the definition (C.27) of variance.

C.4 The geometric and binomial distributions

We can think of a coin flip as an instance of a ***Bernoulli trial***, which is an experiment with only two possible outcomes: ***success***, which occurs with probability p, and ***failure***, which occurs with probability $q = 1 - p$. When we speak of ***Bernoulli trials*** collectively, we mean that the trials are mutually independent and, unless we specifically say otherwise, that each has the same probability p for success. Two

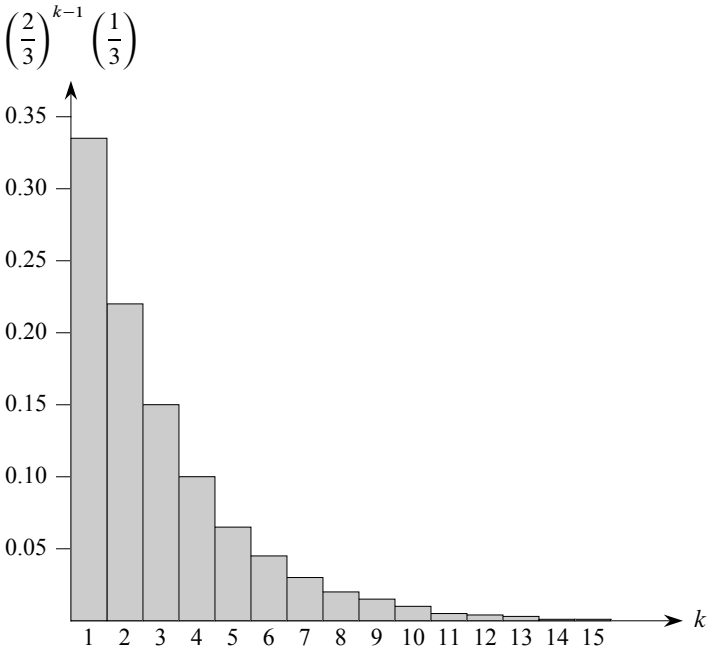

Figure C.1 A geometric distribution with probability $p = 1/3$ of success and a probability $q = 1 - p$ of failure. The expectation of the distribution is $1/p = 3$.

important distributions arise from Bernoulli trials: the geometric distribution and the binomial distribution.

The geometric distribution

Suppose we have a sequence of Bernoulli trials, each with a probability p of success and a probability $q = 1 - p$ of failure. How many trials occur before we obtain a success? Let us define the random variable X be the number of trials needed to obtain a success. Then X has values in the range $\{1, 2, \ldots\}$, and for $k \geq 1$,

$$\Pr\{X = k\} = q^{k-1} p \,, \tag{C.31}$$

since we have $k - 1$ failures before the one success. A probability distribution satisfying equation (C.31) is said to be a ***geometric distribution***. Figure C.1 illustrates such a distribution.

Assuming that $q < 1$, we can calculate the expectation of a geometric distribution using identity (A.8):

$$\begin{aligned}
\mathrm{E}[X] &= \sum_{k=1}^{\infty} k q^{k-1} p \\
&= \frac{p}{q} \sum_{k=0}^{\infty} k q^k \\
&= \frac{p}{q} \cdot \frac{q}{(1-q)^2} \\
&= \frac{p}{q} \cdot \frac{q}{p^2} \\
&= 1/p \, . \qquad \text{(C.32)}
\end{aligned}$$

Thus, on average, it takes $1/p$ trials before we obtain a success, an intuitive result. The variance, which can be calculated similarly, but using Exercise A.1-3, is

$$\mathrm{Var}[X] = q/p^2 \, . \qquad \text{(C.33)}$$

As an example, suppose we repeatedly roll two dice until we obtain either a seven or an eleven. Of the 36 possible outcomes, 6 yield a seven and 2 yield an eleven. Thus, the probability of success is $p = 8/36 = 2/9$, and we must roll $1/p = 9/2 = 4.5$ times on average to obtain a seven or eleven.

The binomial distribution

How many successes occur during n Bernoulli trials, where a success occurs with probability p and a failure with probability $q = 1 - p$? Define the random variable X to be the number of successes in n trials. Then X has values in the range $\{0, 1, \ldots, n\}$, and for $k = 0, 1, \ldots, n$,

$$\Pr\{X = k\} = \binom{n}{k} p^k q^{n-k} \, , \qquad \text{(C.34)}$$

since there are $\binom{n}{k}$ ways to pick which k of the n trials are successes, and the probability that each occurs is $p^k q^{n-k}$. A probability distribution satisfying equation (C.34) is said to be a ***binomial distribution***. For convenience, we define the family of binomial distributions using the notation

$$b(k; n, p) = \binom{n}{k} p^k (1-p)^{n-k} \, . \qquad \text{(C.35)}$$

Figure C.2 illustrates a binomial distribution. The name "binomial" comes from the right-hand side of equation (C.34) being the kth term of the expansion of $(p+q)^n$. Consequently, since $p + q = 1$,

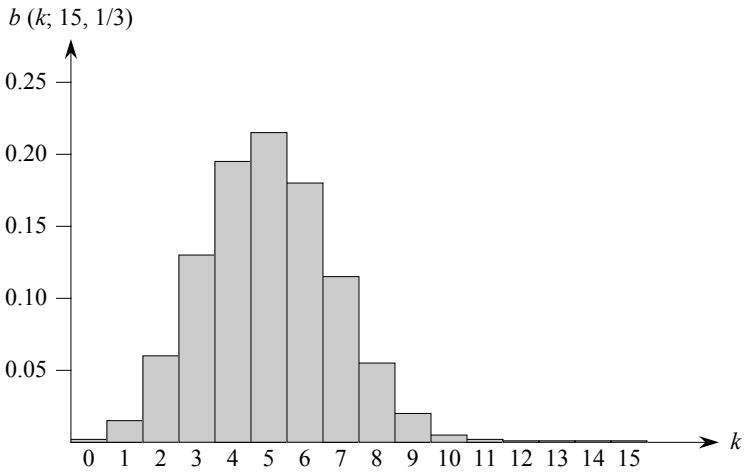

Figure C.2 The binomial distribution $b(k; 15, 1/3)$ resulting from $n = 15$ Bernoulli trials, each with probability $p = 1/3$ of success. The expectation of the distribution is $np = 5$.

$$\sum_{k=0}^{n} b(k; n, p) = 1 , \tag{C.36}$$

as axiom 2 of the probability axioms requires.

We can compute the expectation of a random variable having a binomial distribution from equations (C.8) and (C.36). Let X be a random variable that follows the binomial distribution $b(k; n, p)$, and let $q = 1 - p$. By the definition of expectation, we have

$$\begin{aligned}
\mathrm{E}[X] &= \sum_{k=0}^{n} k \cdot \Pr\{X = k\} \\
&= \sum_{k=0}^{n} k \cdot b(k; n, p) \\
&= \sum_{k=1}^{n} k \binom{n}{k} p^k q^{n-k} \\
&= np \sum_{k=1}^{n} \binom{n-1}{k-1} p^{k-1} q^{n-k} \qquad \text{(by equation (C.8))} \\
&= np \sum_{k=0}^{n-1} \binom{n-1}{k} p^k q^{(n-1)-k}
\end{aligned}$$

$$
\begin{aligned}
&= np \sum_{k=0}^{n-1} b(k; n-1, p) \\
&= np \qquad \text{(by equation (C.36))} \ . \qquad \text{(C.37)}
\end{aligned}
$$

By using the linearity of expectation, we can obtain the same result with substantially less algebra. Let X_i be the random variable describing the number of successes in the ith trial. Then $\mathrm{E}[X_i] = p \cdot 1 + q \cdot 0 = p$, and by linearity of expectation (equation (C.21)), the expected number of successes for n trials is

$$
\begin{aligned}
\mathrm{E}[X] &= \mathrm{E}\left[\sum_{i=1}^{n} X_i\right] \\
&= \sum_{i=1}^{n} \mathrm{E}[X_i] \\
&= \sum_{i=1}^{n} p \\
&= np \ . \qquad \text{(C.38)}
\end{aligned}
$$

We can use the same approach to calculate the variance of the distribution. Using equation (C.27), we have $\mathrm{Var}[X_i] = \mathrm{E}[X_i^2] - \mathrm{E}^2[X_i]$. Since X_i only takes on the values 0 and 1, we have $X_i^2 = X_i$, which implies $\mathrm{E}[X_i^2] = \mathrm{E}[X_i] = p$. Hence,

$$
\mathrm{Var}[X_i] = p - p^2 = p(1-p) = pq \ . \qquad \text{(C.39)}
$$

To compute the variance of X, we take advantage of the independence of the n trials; thus, by equation (C.29),

$$
\begin{aligned}
\mathrm{Var}[X] &= \mathrm{Var}\left[\sum_{i=1}^{n} X_i\right] \\
&= \sum_{i=1}^{n} \mathrm{Var}[X_i] \\
&= \sum_{i=1}^{n} pq \\
&= npq \ . \qquad \text{(C.40)}
\end{aligned}
$$

As Figure C.2 shows, the binomial distribution $b(k; n, p)$ increases with k until it reaches the mean np, and then it decreases. We can prove that the distribution always behaves in this manner by looking at the ratio of successive terms:

$$\begin{aligned}\frac{b(k;n,p)}{b(k-1;n,p)} &= \frac{\binom{n}{k}p^k q^{n-k}}{\binom{n}{k-1}p^{k-1}q^{n-k+1}} \\ &= \frac{n!(k-1)!(n-k+1)!p}{k!(n-k)!n!q} \\ &= \frac{(n-k+1)p}{kq} \\ &= 1+\frac{(n+1)p-k}{kq}\,.\end{aligned} \tag{C.41}$$

This ratio is greater than 1 precisely when $(n+1)p-k$ is positive. Consequently, $b(k;n,p) > b(k-1;n,p)$ for $k < (n+1)p$ (the distribution increases), and $b(k;n,p) < b(k-1;n,p)$ for $k > (n+1)p$ (the distribution decreases). If $k = (n+1)p$ is an integer, then $b(k;n,p) = b(k-1;n,p)$, and so the distribution then has two maxima: at $k = (n+1)p$ and at $k-1 = (n+1)p-1 = np-q$. Otherwise, it attains a maximum at the unique integer k that lies in the range $np-q < k < (n+1)p$.

The following lemma provides an upper bound on the binomial distribution.

Lemma C.1
Let $n \geq 0$, let $0 < p < 1$, let $q = 1-p$, and let $0 \leq k \leq n$. Then

$$b(k;n,p) \leq \left(\frac{np}{k}\right)^k \left(\frac{nq}{n-k}\right)^{n-k}\,.$$

Proof Using equation (C.6), we have

$$\begin{aligned}b(k;n,p) &= \binom{n}{k}p^k q^{n-k} \\ &\leq \left(\frac{n}{k}\right)^k \left(\frac{n}{n-k}\right)^{n-k} p^k q^{n-k} \\ &= \left(\frac{np}{k}\right)^k \left(\frac{nq}{n-k}\right)^{n-k}\,.\end{aligned}$$

■

Exercises

C.4-1
Verify axiom 2 of the probability axioms for the geometric distribution.

C.4-2
How many times on average must we flip 6 fair coins before we obtain 3 heads and 3 tails?

C.4-3
Show that $b(k;n,p) = b(n-k;n,q)$, where $q = 1-p$.

C.4-4
Show that value of the maximum of the binomial distribution $b(k;n,p)$ is approximately $1/\sqrt{2\pi npq}$, where $q = 1-p$.

C.4-5 ⋆
Show that the probability of no successes in n Bernoulli trials, each with probability $p = 1/n$, is approximately $1/e$. Show that the probability of exactly one success is also approximately $1/e$.

C.4-6 ⋆
Professor Rosencrantz flips a fair coin n times, and so does Professor Guildenstern. Show that the probability that they get the same number of heads is $\binom{2n}{n}/4^n$. (*Hint:* For Professor Rosencrantz, call a head a success; for Professor Guildenstern, call a tail a success.) Use your argument to verify the identity

$$\sum_{k=0}^{n} \binom{n}{k}^2 = \binom{2n}{n} .$$

C.4-7 ⋆
Show that for $0 \le k \le n$,

$$b(k;n,1/2) \le 2^{n\,H(k/n)-n} ,$$

where $H(x)$ is the entropy function (C.7).

C.4-8 ⋆
Consider n Bernoulli trials, where for $i = 1,2,\ldots,n$, the ith trial has probability p_i of success, and let X be the random variable denoting the total number of successes. Let $p \ge p_i$ for all $i = 1,2,\ldots,n$. Prove that for $1 \le k \le n$,

$$\Pr\{X < k\} \ge \sum_{i=0}^{k-1} b(i;n,p) .$$

C.4-9 ⋆
Let X be the random variable for the total number of successes in a set A of n Bernoulli trials, where the ith trial has a probability p_i of success, and let X' be the random variable for the total number of successes in a second set A' of n Bernoulli trials, where the ith trial has a probability $p'_i \ge p_i$ of success. Prove that for $0 \le k \le n$,

$$\Pr\{X' \geq k\} \geq \Pr\{X \geq k\} \ .$$

(*Hint:* Show how to obtain the Bernoulli trials in A' by an experiment involving the trials of A, and use the result of Exercise C.3-7.)

⋆ C.5 The tails of the binomial distribution

The probability of having at least, or at most, k successes in n Bernoulli trials, each with probability p of success, is often of more interest than the probability of having exactly k successes. In this section, we investigate the ***tails*** of the binomial distribution: the two regions of the distribution $b(k; n, p)$ that are far from the mean np. We shall prove several important bounds on (the sum of all terms in) a tail.

We first provide a bound on the right tail of the distribution $b(k; n, p)$. We can determine bounds on the left tail by inverting the roles of successes and failures.

Theorem C.2
Consider a sequence of n Bernoulli trials, where success occurs with probability p. Let X be the random variable denoting the total number of successes. Then for $0 \leq k \leq n$, the probability of at least k successes is

$$\begin{aligned}\Pr\{X \geq k\} &= \sum_{i=k}^{n} b(i; n, p) \\ &\leq \binom{n}{k} p^k \ .\end{aligned}$$

Proof For $S \subseteq \{1, 2, \ldots, n\}$, we let A_S denote the event that the ith trial is a success for every $i \in S$. Clearly $\Pr\{A_S\} = p^k$ if $|S| = k$. We have

$$\begin{aligned}\Pr\{X \geq k\} &= \Pr\{\text{there exists } S \subseteq \{1, 2, \ldots, n\} : |S| = k \text{ and } A_S\} \\ &= \Pr\left\{\bigcup_{S \subseteq \{1,2,\ldots,n\} : |S| = k} A_S\right\} \\ &\leq \sum_{S \subseteq \{1,2,\ldots,n\} : |S| = k} \Pr\{A_S\} \qquad \text{(by inequality (C.19))} \\ &= \binom{n}{k} p^k \ .\end{aligned}$$

■

The following corollary restates the theorem for the left tail of the binomial distribution. In general, we shall leave it to you to adapt the proofs from one tail to the other.

Corollary C.3
Consider a sequence of n Bernoulli trials, where success occurs with probability p. If X is the random variable denoting the total number of successes, then for $0 \le k \le n$, the probability of at most k successes is

$$\begin{aligned}\Pr\{X \le k\} &= \sum_{i=0}^{k} b(i; n, p) \\ &\le \binom{n}{n-k}(1-p)^{n-k} \\ &= \binom{n}{k}(1-p)^{n-k} .\end{aligned}$$

■

Our next bound concerns the left tail of the binomial distribution. Its corollary shows that, far from the mean, the left tail diminishes exponentially.

Theorem C.4
Consider a sequence of n Bernoulli trials, where success occurs with probability p and failure with probability $q = 1 - p$. Let X be the random variable denoting the total number of successes. Then for $0 < k < np$, the probability of fewer than k successes is

$$\begin{aligned}\Pr\{X < k\} &= \sum_{i=0}^{k-1} b(i; n, p) \\ &< \frac{kq}{np - k} b(k; n, p) .\end{aligned}$$

Proof We bound the series $\sum_{i=0}^{k-1} b(i; n, p)$ by a geometric series using the technique from Section A.2, page 1151. For $i = 1, 2, \ldots, k$, we have from equation (C.41),

$$\begin{aligned}\frac{b(i-1; n, p)}{b(i; n, p)} &= \frac{iq}{(n-i+1)p} \\ &< \frac{iq}{(n-i)p} \\ &\le \frac{kq}{(n-k)p} .\end{aligned}$$

If we let

$$\begin{aligned} x &= \frac{kq}{(n-k)p} \\ &< \frac{kq}{(n-np)p} \\ &= \frac{kq}{nqp} \\ &= \frac{k}{np} \\ &< 1 , \end{aligned}$$

it follows that

$$b(i-1;n,p) < x\, b(i;n,p)$$

for $0 < i \le k$. Iteratively applying this inequality $k-i$ times, we obtain

$$b(i;n,p) < x^{k-i}\, b(k;n,p)$$

for $0 \le i < k$, and hence

$$\begin{aligned} \sum_{i=0}^{k-1} b(i;n,p) &< \sum_{i=0}^{k-1} x^{k-i} b(k;n,p) \\ &< b(k;n,p) \sum_{i=1}^{\infty} x^i \\ &= \frac{x}{1-x}\, b(k;n,p) \\ &= \frac{kq}{np-k}\, b(k;n,p) . \end{aligned}$$

■

Corollary C.5

Consider a sequence of n Bernoulli trials, where success occurs with probability p and failure with probability $q = 1-p$. Then for $0 < k \le np/2$, the probability of fewer than k successes is less than one half of the probability of fewer than $k+1$ successes.

Proof Because $k \le np/2$, we have

$$\frac{kq}{np-k} \le \frac{(np/2)q}{np-(np/2)}$$

$$\begin{aligned} &= \frac{(np/2)q}{np/2} \\ &\leq 1 , \end{aligned} \tag{C.42}$$

since $q \leq 1$. Letting X be the random variable denoting the number of successes, Theorem C.4 and inequality (C.42) imply that the probability of fewer than k successes is

$$\Pr\{X < k\} = \sum_{i=0}^{k-1} b(i; n, p) < b(k; n, p) .$$

Thus we have

$$\begin{aligned} \frac{\Pr\{X < k\}}{\Pr\{X < k+1\}} &= \frac{\sum_{i=0}^{k-1} b(i; n, p)}{\sum_{i=0}^{k} b(i; n, p)} \\ &= \frac{\sum_{i=0}^{k-1} b(i; n, p)}{\sum_{i=0}^{k-1} b(i; n, p) + b(k; n, p)} \\ &< 1/2 , \end{aligned}$$

since $\sum_{i=0}^{k-1} b(i; n, p) < b(k; n, p)$. ■

Bounds on the right tail follow similarly. Exercise C.5-2 asks you to prove them.

Corollary C.6

Consider a sequence of n Bernoulli trials, where success occurs with probability p. Let X be the random variable denoting the total number of successes. Then for $np < k < n$, the probability of more than k successes is

$$\begin{aligned} \Pr\{X > k\} &= \sum_{i=k+1}^{n} b(i; n, p) \\ &< \frac{(n-k)p}{k-np} b(k; n, p) . \end{aligned}$$

■

Corollary C.7

Consider a sequence of n Bernoulli trials, where success occurs with probability p and failure with probability $q = 1 - p$. Then for $(np + n)/2 < k < n$, the probability of more than k successes is less than one half of the probability of more than $k - 1$ successes. ■

The next theorem considers n Bernoulli trials, each with a probability p_i of success, for $i = 1, 2, \ldots, n$. As the subsequent corollary shows, we can use the

theorem to provide a bound on the right tail of the binomial distribution by setting $p_i = p$ for each trial.

Theorem C.8

Consider a sequence of n Bernoulli trials, where in the ith trial, for $i = 1, 2, \ldots, n$, success occurs with probability p_i and failure occurs with probability $q_i = 1 - p_i$. Let X be the random variable describing the total number of successes, and let $\mu = \mathrm{E}[X]$. Then for $r > \mu$,

$$\Pr\{X - \mu \geq r\} \leq \left(\frac{\mu e}{r}\right)^r .$$

Proof Since for any $\alpha > 0$, the function $e^{\alpha x}$ is strictly increasing in x,

$$\Pr\{X - \mu \geq r\} = \Pr\left\{e^{\alpha(X-\mu)} \geq e^{\alpha r}\right\} , \tag{C.43}$$

where we will determine α later. Using Markov's inequality (C.30), we obtain

$$\Pr\left\{e^{\alpha(X-\mu)} \geq e^{\alpha r}\right\} \leq \mathrm{E}\left[e^{\alpha(X-\mu)}\right] e^{-\alpha r} . \tag{C.44}$$

The bulk of the proof consists of bounding $\mathrm{E}\left[e^{\alpha(X-\mu)}\right]$ and substituting a suitable value for α in inequality (C.44). First, we evaluate $\mathrm{E}\left[e^{\alpha(X-\mu)}\right]$. Using the technique of indicator random variables (see Section 5.2), let $X_i = \mathrm{I}\{\text{the } i\text{th Bernoulli trial is a success}\}$ for $i = 1, 2, \ldots, n$; that is, X_i is the random variable that is 1 if the ith Bernoulli trial is a success and 0 if it is a failure. Thus,

$$X = \sum_{i=1}^{n} X_i ,$$

and by linearity of expectation,

$$\mu = \mathrm{E}[X] = \mathrm{E}\left[\sum_{i=1}^{n} X_i\right] = \sum_{i=1}^{n} \mathrm{E}[X_i] = \sum_{i=1}^{n} p_i ,$$

which implies

$$X - \mu = \sum_{i=1}^{n} (X_i - p_i) .$$

To evaluate $\mathrm{E}\left[e^{\alpha(X-\mu)}\right]$, we substitute for $X - \mu$, obtaining

$$\begin{aligned}
\mathrm{E}\left[e^{\alpha(X-\mu)}\right] &= \mathrm{E}\left[e^{\alpha \sum_{i=1}^{n}(X_i - p_i)}\right] \\
&= \mathrm{E}\left[\prod_{i=1}^{n} e^{\alpha(X_i - p_i)}\right] \\
&= \prod_{i=1}^{n} \mathrm{E}\left[e^{\alpha(X_i - p_i)}\right] ,
\end{aligned}$$

which follows from (C.24), since the mutual independence of the random variables X_i implies the mutual independence of the random variables $e^{\alpha(X_i - p_i)}$ (see Exercise C.3-5). By the definition of expectation,

$$\begin{aligned} \mathrm{E}\left[e^{\alpha(X_i - p_i)}\right] &= e^{\alpha(1-p_i)} p_i + e^{\alpha(0-p_i)} q_i \\ &= p_i e^{\alpha q_i} + q_i e^{-\alpha p_i} \\ &\le p_i e^{\alpha} + 1 \\ &\le \exp(p_i e^{\alpha}) , \end{aligned} \tag{C.45}$$

where $\exp(x)$ denotes the exponential function: $\exp(x) = e^x$. (Inequality (C.45) follows from the inequalities $\alpha > 0$, $q_i \le 1$, $e^{\alpha q_i} \le e^{\alpha}$, and $e^{-\alpha p_i} \le 1$, and the last line follows from inequality (3.12).) Consequently,

$$\begin{aligned} \mathrm{E}\left[e^{\alpha(X-\mu)}\right] &= \prod_{i=1}^{n} \mathrm{E}\left[e^{\alpha(X_i - p_i)}\right] \\ &\le \prod_{i=1}^{n} \exp(p_i e^{\alpha}) \\ &= \exp\left(\sum_{i=1}^{n} p_i e^{\alpha}\right) \\ &= \exp(\mu e^{\alpha}) , \end{aligned} \tag{C.46}$$

since $\mu = \sum_{i=1}^{n} p_i$. Therefore, from equation (C.43) and inequalities (C.44) and (C.46), it follows that

$$\Pr\{X - \mu \ge r\} \le \exp(\mu e^{\alpha} - \alpha r) . \tag{C.47}$$

Choosing $\alpha = \ln(r/\mu)$ (see Exercise C.5-7), we obtain

$$\begin{aligned} \Pr\{X - \mu \ge r\} &\le \exp(\mu e^{\ln(r/\mu)} - r \ln(r/\mu)) \\ &= \exp(r - r \ln(r/\mu)) \\ &= \frac{e^r}{(r/\mu)^r} \\ &= \left(\frac{\mu e}{r}\right)^r . \end{aligned}$$

■

When applied to Bernoulli trials in which each trial has the same probability of success, Theorem C.8 yields the following corollary bounding the right tail of a binomial distribution.

Corollary C.9
Consider a sequence of n Bernoulli trials, where in each trial success occurs with probability p and failure occurs with probability $q = 1 - p$. Then for $r > np$,

$$\begin{aligned}\Pr\{X - np \geq r\} &= \sum_{k=\lceil np+r \rceil}^{n} b(k; n, p) \\ &\leq \left(\frac{npe}{r}\right)^r .\end{aligned}$$

Proof By equation (C.37), we have $\mu = \mathrm{E}[X] = np$. ∎

Exercises

C.5-1 ⋆
Which is less likely: obtaining no heads when you flip a fair coin n times, or obtaining fewer than n heads when you flip the coin $4n$ times?

C.5-2 ⋆
Prove Corollaries C.6 and C.7.

C.5-3 ⋆
Show that

$$\sum_{i=0}^{k-1} \binom{n}{i} a^i < (a+1)^n \frac{k}{na - k(a+1)} b(k; n, a/(a+1))$$

for all $a > 0$ and all k such that $0 < k < na/(a+1)$.

C.5-4 ⋆
Prove that if $0 < k < np$, where $0 < p < 1$ and $q = 1 - p$, then

$$\sum_{i=0}^{k-1} p^i q^{n-i} < \frac{kq}{np - k} \left(\frac{np}{k}\right)^k \left(\frac{nq}{n-k}\right)^{n-k} .$$

C.5-5 ⋆
Use Theorem C.8 to show that

$$\Pr\{\mu - X \geq r\} \leq \left(\frac{(n-\mu)e}{r}\right)^r$$

for $r > n - \mu$. Similarly, use Corollary C.9 to show that

$$\Pr\{np - X \geq r\} \leq \left(\frac{nqe}{r}\right)^r$$

for $r > n - np$.

C.5-6 ⋆

Consider a sequence of n Bernoulli trials, where in the ith trial, for $i = 1, 2, \ldots, n$, success occurs with probability p_i and failure occurs with probability $q_i = 1 - p_i$. Let X be the random variable describing the total number of successes, and let $\mu = \mathrm{E}[X]$. Show that for $r \geq 0$,

$$\Pr\{X - \mu \geq r\} \leq e^{-r^2/2n} .$$

(*Hint:* Prove that $p_i e^{\alpha q_i} + q_i e^{-\alpha p_i} \leq e^{\alpha^2/2}$. Then follow the outline of the proof of Theorem C.8, using this inequality in place of inequality (C.45).)

C.5-7 ⋆

Show that choosing $\alpha = \ln(r/\mu)$ minimizes the right-hand side of inequality (C.47).

Problems

C-1 Balls and bins

In this problem, we investigate the effect of various assumptions on the number of ways of placing n balls into b distinct bins.

a. Suppose that the n balls are distinct and that their order within a bin does not matter. Argue that the number of ways of placing the balls in the bins is b^n.

b. Suppose that the balls are distinct and that the balls in each bin are ordered. Prove that there are exactly $(b + n - 1)!/(b - 1)!$ ways to place the balls in the bins. (*Hint:* Consider the number of ways of arranging n distinct balls and $b - 1$ indistinguishable sticks in a row.)

c. Suppose that the balls are identical, and hence their order within a bin does not matter. Show that the number of ways of placing the balls in the bins is $\binom{b+n-1}{n}$. (*Hint:* Of the arrangements in part (b), how many are repeated if the balls are made identical?)

d. Suppose that the balls are identical and that no bin may contain more than one ball, so that $n \leq b$. Show that the number of ways of placing the balls is $\binom{b}{n}$.

e. Suppose that the balls are identical and that no bin may be left empty. Assuming that $n \geq b$, show that the number of ways of placing the balls is $\binom{n-1}{b-1}$.

Appendix notes

The first general methods for solving probability problems were discussed in a famous correspondence between B. Pascal and P. de Fermat, which began in 1654, and in a book by C. Huygens in 1657. Rigorous probability theory began with the work of J. Bernoulli in 1713 and A. De Moivre in 1730. Further developments of the theory were provided by P.-S. Laplace, S.-D. Poisson, and C. F. Gauss.

Sums of random variables were originally studied by P. L. Chebyshev and A. A. Markov. A. N. Kolmogorov axiomatized probability theory in 1933. Chernoff [66] and Hoeffding [173] provided bounds on the tails of distributions. Seminal work in random combinatorial structures was done by P. Erdős.

Knuth [209] and Liu [237] are good references for elementary combinatorics and counting. Standard textbooks such as Billingsley [46], Chung [67], Drake [95], Feller [104], and Rozanov [300] offer comprehensive introductions to probability.

D Matrices

Matrices arise in numerous applications, including, but by no means limited to, scientific computing. If you have seen matrices before, much of the material in this appendix will be familiar to you, but some of it might be new. Section D.1 covers basic matrix definitions and operations, and Section D.2 presents some basic matrix properties.

D.1 Matrices and matrix operations

In this section, we review some basic concepts of matrix theory and some fundamental properties of matrices.

Matrices and vectors

A ***matrix*** is a rectangular array of numbers. For example,

$$\begin{aligned} A &= \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{pmatrix} \\ &= \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix} \end{aligned} \tag{D.1}$$

is a 2×3 matrix $A = (a_{ij})$, where for $i = 1, 2$ and $j = 1, 2, 3$, we denote the element of the matrix in row i and column j by a_{ij}. We use uppercase letters to denote matrices and corresponding subscripted lowercase letters to denote their elements. We denote the set of all $m \times n$ matrices with real-valued entries by $\mathbb{R}^{m \times n}$ and, in general, the set of $m \times n$ matrices with entries drawn from a set S by $S^{m \times n}$.

The ***transpose*** of a matrix A is the matrix A^{T} obtained by exchanging the rows and columns of A. For the matrix A of equation (D.1),

$$A^{\mathrm{T}} = \begin{pmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{pmatrix}.$$

A ***vector*** is a one-dimensional array of numbers. For example,

$$x = \begin{pmatrix} 2 \\ 3 \\ 5 \end{pmatrix}$$

is a vector of size 3. We sometimes call a vector of length n an ***n-vector***. We use lowercase letters to denote vectors, and we denote the ith element of a size-n vector x by x_i, for $i = 1, 2, \ldots, n$. We take the standard form of a vector to be as a ***column vector*** equivalent to an $n \times 1$ matrix; the corresponding ***row vector*** is obtained by taking the transpose:

$$x^{\mathrm{T}} = \begin{pmatrix} 2 & 3 & 5 \end{pmatrix}.$$

The ***unit vector*** e_i is the vector whose ith element is 1 and all of whose other elements are 0. Usually, the size of a unit vector is clear from the context.

A ***zero matrix*** is a matrix all of whose entries are 0. Such a matrix is often denoted 0, since the ambiguity between the number 0 and a matrix of 0s is usually easily resolved from context. If a matrix of 0s is intended, then the size of the matrix also needs to be derived from the context.

Square matrices

Square $n \times n$ matrices arise frequently. Several special cases of square matrices are of particular interest:

1. A ***diagonal matrix*** has $a_{ij} = 0$ whenever $i \neq j$. Because all of the off-diagonal elements are zero, we can specify the matrix by listing the elements along the diagonal:

$$\mathrm{diag}(a_{11}, a_{22}, \ldots, a_{nn}) = \begin{pmatrix} a_{11} & 0 & \ldots & 0 \\ 0 & a_{22} & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & a_{nn} \end{pmatrix}.$$

2. The $n \times n$ ***identity matrix*** I_n is a diagonal matrix with 1s along the diagonal:

$$\begin{aligned} I_n &= \mathrm{diag}(1, 1, \ldots, 1) \\ &= \begin{pmatrix} 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 1 \end{pmatrix}. \end{aligned}$$

When I appears without a subscript, we derive its size from the context. The ith column of an identity matrix is the unit vector e_i.

3. A ***tridiagonal matrix*** T is one for which $t_{ij} = 0$ if $|i - j| > 1$. Nonzero entries appear only on the main diagonal, immediately above the main diagonal ($t_{i,i+1}$ for $i = 1, 2, \ldots, n-1$), or immediately below the main diagonal ($t_{i+1,i}$ for $i = 1, 2, \ldots, n-1$):

$$T = \begin{pmatrix} t_{11} & t_{12} & 0 & 0 & \ldots & 0 & 0 & 0 \\ t_{21} & t_{22} & t_{23} & 0 & \ldots & 0 & 0 & 0 \\ 0 & t_{32} & t_{33} & t_{34} & \ldots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \ldots & t_{n-2,n-2} & t_{n-2,n-1} & 0 \\ 0 & 0 & 0 & 0 & \ldots & t_{n-1,n-2} & t_{n-1,n-1} & t_{n-1,n} \\ 0 & 0 & 0 & 0 & \ldots & 0 & t_{n,n-1} & t_{nn} \end{pmatrix} .$$

4. An ***upper-triangular matrix*** U is one for which $u_{ij} = 0$ if $i > j$. All entries below the diagonal are zero:

$$U = \begin{pmatrix} u_{11} & u_{12} & \ldots & u_{1n} \\ 0 & u_{22} & \ldots & u_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & u_{nn} \end{pmatrix} .$$

An upper-triangular matrix is ***unit upper-triangular*** if it has all 1s along the diagonal.

5. A ***lower-triangular matrix*** L is one for which $l_{ij} = 0$ if $i < j$. All entries above the diagonal are zero:

$$L = \begin{pmatrix} l_{11} & 0 & \ldots & 0 \\ l_{21} & l_{22} & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & \ldots & l_{nn} \end{pmatrix} .$$

A lower-triangular matrix is ***unit lower-triangular*** if it has all 1s along the diagonal.

6. A ***permutation matrix*** P has exactly one 1 in each row or column, and 0s elsewhere. An example of a permutation matrix is

$$P = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} .$$

   Such a matrix is called a permutation matrix because multiplying a vector x by a permutation matrix has the effect of permuting (rearranging) the elements of x. Exercise D.1-4 explores additional properties of permutation matrices.

7. A ***symmetric matrix*** A satisfies the condition $A = A^{\mathrm{T}}$. For example,

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 6 & 4 \\ 3 & 4 & 5 \end{pmatrix}$$

   is a symmetric matrix.

Basic matrix operations

The elements of a matrix or vector are numbers from a number system, such as the real numbers, the complex numbers, or integers modulo a prime. The number system defines how to add and multiply numbers. We can extend these definitions to encompass addition and multiplication of matrices.

We define ***matrix addition*** as follows. If $A = (a_{ij})$ and $B = (b_{ij})$ are $m \times n$ matrices, then their matrix sum $C = (c_{ij}) = A + B$ is the $m \times n$ matrix defined by

$$c_{ij} = a_{ij} + b_{ij}$$

for $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n$. That is, matrix addition is performed componentwise. A zero matrix is the identity for matrix addition:

$$A + 0 = A = 0 + A .$$

If λ is a number and $A = (a_{ij})$ is a matrix, then $\lambda A = (\lambda a_{ij})$ is the ***scalar multiple*** of A obtained by multiplying each of its elements by λ. As a special case, we define the ***negative*** of a matrix $A = (a_{ij})$ to be $-1 \cdot A = -A$, so that the ijth entry of $-A$ is $-a_{ij}$. Thus,

$$A + (-A) = 0 = (-A) + A .$$

We use the negative of a matrix to define ***matrix subtraction***: $A - B = A + (-B)$.

We define ***matrix multiplication*** as follows. We start with two matrices A and B that are ***compatible*** in the sense that the number of columns of A equals the number of rows of B. (In general, an expression containing a matrix product AB is always assumed to imply that matrices A and B are compatible.) If $A = (a_{ik})$ is an $m \times n$ matrix and $B = (b_{kj})$ is an $n \times p$ matrix, then their matrix product $C = AB$ is the $m \times p$ matrix $C = (c_{ij})$, where

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj} \tag{D.2}$$

for $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, p$. The procedure SQUARE-MATRIX-MULTIPLY in Section 4.2 implements matrix multiplication in the straightforward manner based on equation (D.2), assuming that the matrices are square: $m = n = p$. To multiply $n \times n$ matrices, SQUARE-MATRIX-MULTIPLY performs n^3 multiplications and $n^2(n-1)$ additions, and so its running time is $\Theta(n^3)$.

Matrices have many (but not all) of the algebraic properties typical of numbers. Identity matrices are identities for matrix multiplication:

$$I_m A = A I_n = A$$

for any $m \times n$ matrix A. Multiplying by a zero matrix gives a zero matrix:

$$A\,0 = 0\,.$$

Matrix multiplication is associative:

$$A(BC) = (AB)C$$

for compatible matrices A, B, and C. Matrix multiplication distributes over addition:

$$\begin{aligned} A(B + C) &= AB + AC\,, \\ (B + C)D &= BD + CD\,. \end{aligned}$$

For $n > 1$, multiplication of $n \times n$ matrices is not commutative. For example, if $A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ and $B = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$, then

$$AB = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

and

$$BA = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

We define matrix-vector products or vector-vector products as if the vector were the equivalent $n \times 1$ matrix (or a $1 \times n$ matrix, in the case of a row vector). Thus, if A is an $m \times n$ matrix and x is an n-vector, then Ax is an m-vector. If x and y are n-vectors, then

$$x^{\mathrm{T}} y = \sum_{i=1}^{n} x_i y_i$$

is a number (actually a 1×1 matrix) called the ***inner product*** of x and y. The matrix $x y^{\mathrm{T}}$ is an $n \times n$ matrix Z called the ***outer product*** of x and y, with $z_{ij} = x_i y_j$. The ***(euclidean) norm*** $\|x\|$ of an n-vector x is defined by

$$\begin{aligned} \|x\| &= (x_1^2 + x_2^2 + \cdots + x_n^2)^{1/2} \\ &= (x^{\mathrm{T}} x)^{1/2} . \end{aligned}$$

Thus, the norm of x is its length in n-dimensional euclidean space.

Exercises

D.1-1
Show that if A and B are symmetric $n \times n$ matrices, then so are $A + B$ and $A - B$.

D.1-2
Prove that $(AB)^{\mathrm{T}} = B^{\mathrm{T}} A^{\mathrm{T}}$ and that $A^{\mathrm{T}} A$ is always a symmetric matrix.

D.1-3
Prove that the product of two lower-triangular matrices is lower-triangular.

D.1-4
Prove that if P is an $n \times n$ permutation matrix and A is an $n \times n$ matrix, then the matrix product PA is A with its rows permuted, and the matrix product AP is A with its columns permuted. Prove that the product of two permutation matrices is a permutation matrix.

D.2 Basic matrix properties

In this section, we define some basic properties pertaining to matrices: inverses, linear dependence and independence, rank, and determinants. We also define the class of positive-definite matrices.

Matrix inverses, ranks, and determinants

We define the ***inverse*** of an $n \times n$ matrix A to be the $n \times n$ matrix, denoted A^{-1} (if it exists), such that $AA^{-1} = I_n = A^{-1}A$. For example,

$$\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}^{-1} = \begin{pmatrix} 0 & 1 \\ 1 & -1 \end{pmatrix} .$$

Many nonzero $n \times n$ matrices do not have inverses. A matrix without an inverse is called ***noninvertible***, or ***singular***. An example of a nonzero singular matrix is

$$\begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix} .$$

If a matrix has an inverse, it is called ***invertible***, or ***nonsingular***. Matrix inverses, when they exist, are unique. (See Exercise D.2-1.) If A and B are nonsingular $n \times n$ matrices, then

$$(BA)^{-1} = A^{-1}B^{-1} .$$

The inverse operation commutes with the transpose operation:

$$(A^{-1})^{\mathrm{T}} = (A^{\mathrm{T}})^{-1} .$$

The vectors $x_1, x_2, \ldots, x_n$ are ***linearly dependent*** if there exist coefficients $c_1, c_2, \ldots, c_n$, not all of which are zero, such that $c_1x_1 + c_2x_2 + \cdots + c_nx_n = 0$. The row vectors $x_1 = (\,1 \quad 2 \quad 3\,)$, $x_2 = (\,2 \quad 6 \quad 4\,)$, and $x_3 = (\,4 \quad 11 \quad 9\,)$ are linearly dependent, for example, since $2x_1 + 3x_2 - 2x_3 = 0$. If vectors are not linearly dependent, they are ***linearly independent***. For example, the columns of an identity matrix are linearly independent.

The ***column rank*** of a nonzero $m \times n$ matrix A is the size of the largest set of linearly independent columns of A. Similarly, the ***row rank*** of A is the size of the largest set of linearly independent rows of A. A fundamental property of any matrix A is that its row rank always equals its column rank, so that we can simply refer to the ***rank*** of A. The rank of an $m \times n$ matrix is an integer between 0 and $\min(m, n)$, inclusive. (The rank of a zero matrix is 0, and the rank of an $n \times n$ identity matrix is n.) An alternate, but equivalent and often more useful, definition is that the rank of a nonzero $m \times n$ matrix A is the smallest number r such that there exist matrices B and C of respective sizes $m \times r$ and $r \times n$ such that

$$A = BC .$$

A square $n \times n$ matrix has ***full rank*** if its rank is n. An $m \times n$ matrix has ***full column rank*** if its rank is n. The following theorem gives a fundamental property of ranks.

Theorem D.1
A square matrix has full rank if and only if it is nonsingular. ■

A ***null vector*** for a matrix A is a nonzero vector x such that $Ax = 0$. The following theorem (whose proof is left as Exercise D.2-7) and its corollary relate the notions of column rank and singularity to null vectors.

Theorem D.2
A matrix A has full column rank if and only if it does not have a null vector. ■

Corollary D.3
A square matrix A is singular if and only if it has a null vector. ■

The ijth ***minor*** of an $n \times n$ matrix A, for $n > 1$, is the $(n-1) \times (n-1)$ matrix $A_{[ij]}$ obtained by deleting the ith row and jth column of A. We define the ***determinant*** of an $n \times n$ matrix A recursively in terms of its minors by

$$\det(A) = \begin{cases} a_{11} & \text{if } n = 1 , \\ \sum_{j=1}^{n} (-1)^{1+j} a_{1j} \det(A_{[1j]}) & \text{if } n > 1 . \end{cases}$$

The term $(-1)^{i+j} \det(A_{[ij]})$ is known as the ***cofactor*** of the element a_{ij}.

The following theorems, whose proofs are omitted here, express fundamental properties of the determinant.

Theorem D.4 (Determinant properties)
The determinant of a square matrix A has the following properties:

- If any row or any column of A is zero, then $\det(A) = 0$.
- The determinant of A is multiplied by λ if the entries of any one row (or any one column) of A are all multiplied by λ.
- The determinant of A is unchanged if the entries in one row (respectively, column) are added to those in another row (respectively, column).
- The determinant of A equals the determinant of A^{T}.
- The determinant of A is multiplied by -1 if any two rows (or any two columns) are exchanged.

Also, for any square matrices A and B, we have $\det(AB) = \det(A) \det(B)$. ■

Theorem D.5
An $n \times n$ matrix A is singular if and only if $\det(A) = 0$. ■

Positive-definite matrices

Positive-definite matrices play an important role in many applications. An $n \times n$ matrix A is ***positive-definite*** if $x^{\mathrm{T}}Ax > 0$ for all n-vectors $x \neq 0$. For example, the identity matrix is positive-definite, since for any nonzero vector $x = (\, x_1 \;\; x_2 \;\; \cdots \;\; x_n \,)^{\mathrm{T}}$,

$$\begin{aligned} x^{\mathrm{T}} I_n x &= x^{\mathrm{T}} x \\ &= \sum_{i=1}^{n} x_i^2 \\ &> 0 \,. \end{aligned}$$

Matrices that arise in applications are often positive-definite due to the following theorem.

Theorem D.6
For any matrix A with full column rank, the matrix $A^{\mathrm{T}}A$ is positive-definite.

Proof We must show that $x^{\mathrm{T}}(A^{\mathrm{T}}A)x > 0$ for any nonzero vector x. For any vector x,

$$\begin{aligned} x^{\mathrm{T}}(A^{\mathrm{T}}A)x &= (Ax)^{\mathrm{T}}(Ax) \quad \text{(by Exercise D.1-2)} \\ &= \|Ax\|^2 \,. \end{aligned}$$

Note that $\|Ax\|^2$ is just the sum of the squares of the elements of the vector Ax. Therefore, $\|Ax\|^2 \geq 0$. If $\|Ax\|^2 = 0$, every element of Ax is 0, which is to say $Ax = 0$. Since A has full column rank, $Ax = 0$ implies $x = 0$, by Theorem D.2. Hence, $A^{\mathrm{T}}A$ is positive-definite. ■

Section 28.3 explores other properties of positive-definite matrices.

Exercises

D.2-1
Prove that matrix inverses are unique, that is, if B and C are inverses of A, then $B = C$.

D.2-2
Prove that the determinant of a lower-triangular or upper-triangular matrix is equal to the product of its diagonal elements. Prove that the inverse of a lower-triangular matrix, if it exists, is lower-triangular.

D.2-3
Prove that if P is a permutation matrix, then P is invertible, its inverse is P^{T}, and P^{T} is a permutation matrix.

D.2-4
Let A and B be $n \times n$ matrices such that $AB = I$. Prove that if A' is obtained from A by adding row j into row i, then subtracting column i from column j of B yields the inverse B' of A'.

D.2-5
Let A be a nonsingular $n \times n$ matrix with complex entries. Show that every entry of A^{-1} is real if and only if every entry of A is real.

D.2-6
Show that if A is a nonsingular, symmetric, $n \times n$ matrix, then A^{-1} is symmetric. Show that if B is an arbitrary $m \times n$ matrix, then the $m \times m$ matrix given by the product BAB^{T} is symmetric.

D.2-7
Prove Theorem D.2. That is, show that a matrix A has full column rank if and only if $Ax = 0$ implies $x = 0$. (*Hint:* Express the linear dependence of one column on the others as a matrix-vector equation.)

D.2-8
Prove that for any two compatible matrices A and B,

$$\mathrm{rank}(AB) \leq \min(\mathrm{rank}(A), \mathrm{rank}(B)) ,$$

where equality holds if either A or B is a nonsingular square matrix. (*Hint:* Use the alternate definition of the rank of a matrix.)

Problems

D-1 Vandermonde matrix
Given numbers $x_0, x_1, \ldots, x_{n-1}$, prove that the determinant of the ***Vandermonde matrix***

$$V(x_0, x_1, \ldots, x_{n-1}) = \begin{pmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^{n-1} \\ 1 & x_1 & x_1^2 & \cdots & x_1^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n-1} & x_{n-1}^2 & \cdots & x_{n-1}^{n-1} \end{pmatrix}$$

is

$$\det(V(x_0, x_1, \ldots, x_{n-1})) = \prod_{0 \le j < k \le n-1} (x_k - x_j) \ .$$

(*Hint:* Multiply column i by $-x_0$ and add it to column $i+1$ for $i = n-1$, $n-2, \ldots, 1$, and then use induction.)

D-2 Permutations defined by matrix-vector multiplication over GF(2)

One class of permutations of the integers in the set $S_n = \{0, 1, 2, \ldots, 2^n - 1\}$ is defined by matrix multiplication over $GF(2)$. For each integer x in S_n, we view its binary representation as an n-bit vector

$$\begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_{n-1} \end{pmatrix} ,$$

where $x = \sum_{i=0}^{n-1} x_i 2^i$. If A is an $n \times n$ matrix in which each entry is either 0 or 1, then we can define a permutation mapping each value x in S_n to the number whose binary representation is the matrix-vector product Ax. Here, we perform all arithmetic over ***GF(2)***: all values are either 0 or 1, and with one exception the usual rules of addition and multiplication apply. The exception is that $1 + 1 = 0$. You can think of arithmetic over $GF(2)$ as being just like regular integer arithmetic, except that you use only the least significant bit.

As an example, for $S_2 = \{0, 1, 2, 3\}$, the matrix

$$A = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$$

defines the following permutation π_A: $\pi_A(0) = 0$, $\pi_A(1) = 3$, $\pi_A(2) = 2$, $\pi_A(3) = 1$. To see why $\pi_A(3) = 1$, observe that, working in $GF(2)$,

$$\begin{aligned} \pi_A(3) &= \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ &= \begin{pmatrix} 1 \cdot 1 + 0 \cdot 1 \\ 1 \cdot 1 + 1 \cdot 1 \end{pmatrix} \\ &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \end{aligned}$$

which is the binary representation of 1.

For the remainder of this problem, we work over $GF(2)$, and all matrix and vector entries are 0 or 1. We define the rank of a 0-1 matrix (a matrix for which each entry is either 0 or 1) over $GF(2)$ the same as for a regular matrix, but with all arithmetic that determines linear independence performed over $GF(2)$. We define the ***range*** of an $n \times n$ 0-1 matrix A by

$$R(A) = \{y : y = Ax \text{ for some } x \in S_n\} ,$$

so that $R(A)$ is the set of numbers in S_n that we can produce by multiplying each value x in S_n by A.

a. If r is the rank of matrix A, prove that $|R(A)| = 2^r$. Conclude that A defines a permutation on S_n only if A has full rank.

For a given $n \times n$ matrix A and a given value $y \in R(A)$, we define the ***preimage*** of y by

$$P(A, y) = \{x : Ax = y\} ,$$

so that $P(A, y)$ is the set of values in S_n that map to y when multiplied by A.

b. If r is the rank of $n \times n$ matrix A and $y \in R(A)$, prove that $|P(A, y)| = 2^{n-r}$.

Let $0 \le m \le n$, and suppose we partition the set S_n into blocks of consecutive numbers, where the ith block consists of the 2^m numbers $i2^m, i2^m + 1, i2^m + 2, \ldots, (i + 1)2^m - 1$. For any subset $S \subseteq S_n$, define $B(S, m)$ to be the set of size-2^m blocks of S_n containing some element of S. As an example, when $n = 3$, $m = 1$, and $S = \{1, 4, 5\}$, then $B(S, m)$ consists of blocks 0 (since 1 is in the 0th block) and 2 (since both 4 and 5 are in block 2).

c. Let r be the rank of the lower left $(n - m) \times m$ submatrix of A, that is, the matrix formed by taking the intersection of the bottom $n - m$ rows and the leftmost m columns of A. Let S be any size-2^m block of S_n, and let $S' = \{y : y = Ax \text{ for some } x \in S\}$. Prove that $|B(S', m)| = 2^r$ and that for each block in $B(S', m)$, exactly 2^{m-r} numbers in S map to that block.

Because multiplying the zero vector by any matrix yields a zero vector, the set of permutations of S_n defined by multiplying by $n \times n$ 0-1 matrices with full rank over $GF(2)$ cannot include all permutations of S_n. Let us extend the class of permutations defined by matrix-vector multiplication to include an additive term, so that $x \in S_n$ maps to $Ax + c$, where c is an n-bit vector and addition is performed over $GF(2)$. For example, when

$$A = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$$

and

$$c = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

we get the following permutation $\pi_{A,c}$: $\pi_{A,c}(0) = 2$, $\pi_{A,c}(1) = 1$, $\pi_{A,c}(2) = 0$, $\pi_{A,c}(3) = 3$. We call any permutation that maps $x \in S_n$ to $Ax + c$, for some $n \times n$ 0-1 matrix A with full rank and some n-bit vector c, a ***linear permutation***.

d. Use a counting argument to show that the number of linear permutations of S_n is much less than the number of permutations of S_n.

e. Give an example of a value of n and a permutation of S_n that cannot be achieved by any linear permutation. (*Hint:* For a given permutation, think about how multiplying a matrix by a unit vector relates to the columns of the matrix.)

Appendix notes

Linear-algebra textbooks provide plenty of background information on matrices. The books by Strang [323, 324] are particularly good.