Linear Algebra and Probability For Computer Science Applications

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Preface

Since computer science (CS) first became an academic discipline, almost 50 years ago, a central question in defining the computer science curriculum has always been, "How much, and what, college-level mathematics does a computer scientist need to know?" As with all curricular questions, the correct answer, of course, is that everyone should know everything about everything; and indeed, if you raise the question over lunch with computer science professors, you will soon hear the familiar lament that the students these days don't know Desargues' theorem and have never heard of a p-adic number. But in view of the limited time available for a degree program, and particularly in view of the fact that every additional math course that a CS student takes is one fewer CS course that he/she has time to take, the conventional wisdom of the field has for the most part converged on the decision that, beyond first-semester calculus, what CS students really need is a one-semester course in "discrete math", a pleasant smorgasbord of logic, set theory, graph theory, and combinatorics. More math than that can be left elective.

From that conventional wisdom, I do not wish to depart; I think it is accurate to say that a discrete math course is indeed largely sufficient mathematical background for a computer scientist working in the "core" areas of the field, such as databases, compilers, operating systems, architecture, and networks; and many computer scientists have had very successful careers knowing little or no more math. Other mathematical issues no doubt arise even in these areas, but peripherally and unsystematically; the computer scientist can learn the math needed as it arises.

However, other areas of computer science, including artificial intelligence, graphics, machine learning, optimization, data mining, computer vision, computational finance, computational biology, bioinformatics, information retrieval, and web search, require a different mathematical background; and the importance of these areas within the field of computer science has steadily increased over the last twenty years. These fields and their subfields of course vary widely in terms of exactly what areas of math they require and at what depth; but three mathematical subjects stand out as particularly important in all or most of these: linear algebra, probability, and multi-variable calculus.

The need for many CS students to learn these subjects is particularly difficult to address in a master's degree program. An undergraduate degree typically involves something like 32 semester courses; it may not be unreasonable to suggest or even to require that they take the undergraduate courses in linear algebra, multi-variable calculus, and probability given by the math department. A master's program, by contrast, typically requires only 10 or 12 courses. Many students entering a master's program have a weak mathematical background, but are eager to get started on those CS courses which have a substantial mathematical prerequisite. One can hardly ask them to delay their computer science work until they have completed 3 or 4 mathematics courses. Moreover, they cannot get graduate credit for undergraduate math courses, and if the math department does offer graduate courses in these areas, the courses are almost certainly too difficult for the CS masters students.

To fill this gap, I created a new course, entitled, vaguely, "Mathematical Techniques for Computer

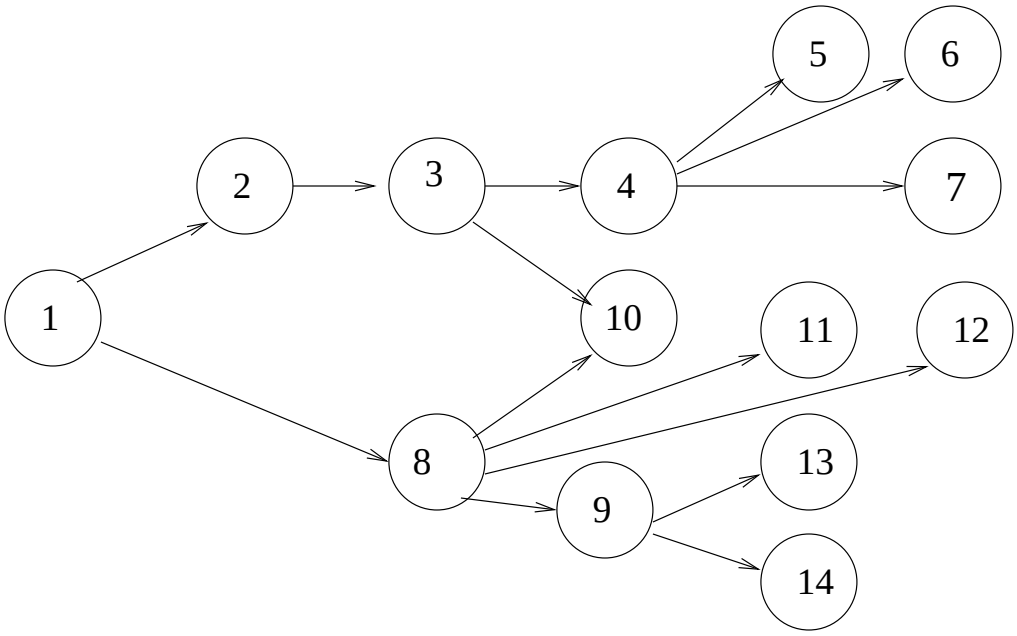


Figure 1: Chapter Dependencies

Science Applications", for the master's program at NYU, giving an intensive introduction to linear algebra and probability, particularly addressed to students with a weak mathematical background. The course has been given once a year, in the fall semester, every year starting in 2009. I taught it myself in 2009 and 2010; it will be taught in 2011 by my colleague Zvi Kedem. This textbook was written specifically for use in this course.

Master's courses in the computer science department at NYU meet fourteen times in a semester, once a week, in two-hour sessions. In my class in 2010, chapters 1 and 2 were covered together in a single lecture; chapters 6 and 9 required two lectures each; chapters 3, 4, 5, 7, 8, 10, 11, 12 and 13, were each covered in a single lecture; and chapter 14 was omitted. About half-way through the class I decided it was necessary to add a recitation section for an additional hour a week; I certainly recommend that.

Multivariable calculus remains a gap and I have not found any practical way of closing it. Obviously, it would not be possible to squeeze all three topics into a single semester, but neither, probably, is it practical to suggest that master's students take two semesters of "Mathematical Techniques".

The course as I teach it involves extensive programming in MATLAB. Correspondingly, the book contains an introductory chapter on MATLAB; discussions in each chapter of the relevant MATLAB functions and features; and many MATLAB assignments.

Figure 1 illustrates the strong dependencies between chapters. (There are also weaker dependencies in which one section of a later chapter depends on material from an earlier chapter; these are not shown.)

There are, of course, plenty of textbooks for probability, and a huge number of textbooks for linear algebra; why write a new one? For one thing, I wanted to have both subjects in a single book; the only other book I have seen that does this is *The Mathematics of Digital Images* by Stuart Hoggar. More importantly, this book is distinguished by being addressed to the computer scientist, rather than the mathematician, physical scientist, or engineer. This affects the *background assumed,* the *choice of topics*, the *examples*, and the *presentation*.

Background. The textbook assumes as little mathematical background as I could manage. Most of the book assumes only high-school mathematics. Complex numbers are nowhere used. In the linear algebra section of the book, calculus is entirely avoided, except in one optional short discussion of Jacobians. In the probability section of the book, this is less feasible, but I have for the most part segregated the sections of the text that do require calculus from those that do not. A basic understanding of integrals is an unavoidable prerequisite for the understanding of continuous probability densities, and an understanding of multiple integrals is a prerequisite for the understanding of the joint distribution of multiple continuous variables.

The issue of mathematical proof in a course of this kind is a difficult one. The book includes the proofs of most, though not all, the theorems that are stated, including a few somewhat lengthy proofs. In chapter 4 on vector spaces, I have in fact split the chapter into two; a first part that contains the minimal material needed for subsequent chapters, with almost no proofs and a second part with more abstract material and more proofs. My own practice in teaching is that in lecture I present some of the proofs that I feel to be enlightening. I do try to keep in mind, however, that, whatever the mathematically-trained instructor may imagine, a proof is not the same as an explanation even for students who are mathematically inclined; for students who are math-averse, a proof bears no relation to an explanation. The textbook includes a number of problems asking the students to write proofs. My own practice in teaching, however, is that I do not assign problems that require proofs. My experience is that the "proofs" produced by students with a weak mathematical background tend to be random sequences of sentences, some of which are true. Unless an instructor is willing to invest substantial effort into teaching what is and is not a valid proof and how one constructs a valid proof, assigning proofs as homework or exam problems is merely frustrating and wearisome for both the student and the grader.

On the other hand, I have assumed some familiarity with basic concepts of computer science. I assume throughout that the student is comfortable writing programs, and I discuss issues such as computational complexity, round-off error, and programming language design (in connection with MATLAB).

Choice of topics: In both parts of the course, the topics included are intended to be those areas that are most important to the computer scientist. These somewhat different from the usual material in the corresponding introductory math classes, where the intended audience is usually math and science students. I have been guided here both by own impression and by discussions with colleagues. In the linear algebra section, I have restricted the discussion to finite-dimensional vectors and matrices over the reals. Determinants are mentioned only briefly as a measure of volume change and handedness change in geometric transformations. I have almost entirely omitted discussion of eigenvalues and eigenvectors, both because they seem to be more important in physics and engineering than in CS applications, and because the theory of eigenvalues really cannot be reasonably presented without using complex eigenvalues. Instead, I have included a discussion of the singular value decomposition, which has more CS applications and involves only real values. I have also included a more extensive discussion of geometric applications and of issues of floating point computation than many standard linear algebra textbooks.

In the probability section, I have included only a minimal discussion of combinatorics, such as counting combinations and permutations. I have also omitted a number of well-known distributions such as the Poisson distribution. On the other hand I have included the inverse power-law "Zipf" distribution, which arises often in CS applications, but is not often discussed in probability textbooks. I have also included discussions of the likelihood interpretation vs. the sample space interpretation of probability and of the basic elements of information theory; and a very rudimentary introduction to basic techniques of statistics.

Examples and presentation: The examples and the programming assignments focus on computer science applications. The applications discussed here are drawn from a wide range of areas of com-

puter science, including computer graphics, computer vision, robotics, natural language processing, web search, machine learning, statistical analysis, game playing, graph theory, scientific computing, decision theory, coding, cryptography, network analysis, data compression, and signal processing There is, no doubt, a bias toward artificial intelligence, particularly natural language processing, and toward geometric problems, partly because of my own interests, partly because these areas lend themselves to simple programs that do interesting things. Likewise, the presentation is geared toward problems that arise in programming and to computer science.

Homework problems are provided at the end of each chapter. These are divided into three categories. **Exercises** are problems that involve a single calculation; some of these can be done by hand, some of these require Matlab. Most of these are short, but a few are quite demanding, such as exercise 10.2, "Compute the Markov model and stationary distribution for Monopoly." **Programming Assignments** require the student to write a MATLAB function with parameters. These vary considerably in difficulty; a few are as short as one line of MATLAB, others require some hundreds of lines. I have not included any assignments that would qualify for a semester project. **Problems** includes everything else; generally "thought problems", particularly proofs.

Course website

The web site for course materials is at http://www.cs.nyu.edu/faculty/davise/MathTechniques/ In particular, MATLAB code discussed in this text can be found here.

Errors, queries, and suggestions for improvements should be emailed to davise@cs.nyu.edu.

Acknowledgements

I am very grateful to my colleagues for their encouragement and suggestions in the development of this course and the writing of this book. I am especially grateful to Michael Overton, who was deeply involved in the design of the linear algebra section of the course, read two drafts of that section of the text, and made many suggestions which greatly enriched it. I have also received valuable suggestions and information from Marsha Berger, Zvi Kedem, Gregory Lawler, Dennis Shasha, Alan Siegel, and Olga Sorkine.

I owe a special debt of gratitude to the students in "Mathematical Techniques for Computer Science Applications" who suffered through early drafts of this text and of many of the assignments, and who gave invaluable feedback.

During part of the writing of this book, I had support from the National Science Foundation on grant #IIS-0534809.

My own introduction to linear algebra and to probability theory came from courses that I took with Bruno Harris in spring 1974 and with the late Gian-Carlo Rota in fall 1975. I hope that this book is a credit to their teaching.

DEDICATION

For my beloved father

Philip J. Davis

who has had a lifelong love of *matrices*,

a profound respect for the workings of *chance,*

and a healthy distrust of the *applications of statistical inference*.

> Consider the recent flight to Mars that put a "laboratory vehicle" on that planet. ... From first to last, the Mars shot would have been impossible without a tremendous underlay of mathematics built into chips and software. It would defy the most knowledgeable historian of mathematics to discover and describe all the mathematics involved.

— Philip Davis, "A Letter to Christina of Denmark," *Newsletter of the European Mathematical Society,* **51**, March 2004, 21-24.

Chapter 1

MATLAB

MATLAB (short for MATrix LABoratory) is a programming language, together with a programming environment, designed to facilitate mathematical calculations and rapid prototyping of mathematical programs. It was created in the late 1970's by Cleve Moler, and has become very popular in the mathematical, scientific, and engineering communities.

MATLAB creates a collection of windows. These may be "docked" – that is, all placed together within a single window — or "undocked".

The most important is the Command window. The user types MATLAB commands into the Command window. The MATLAB interpreter executes the command and prints the value in the Command window. To suppress a print out (useful with a large object), the user can type ; at the end of the command.

The user prompt is in the Command window is >>.
Comments begin with a percent sign % and continue to the end of the line.

In this chapter, we present some basic features of the language. More advanced features, including operations on vectors and matrices, will be discussed in the chapters where the associated math is presented.

All the MATLAB examples in this book were generated using MATLAB 7.8.0 (R2009a).

There are many fine handbooks for MATLAB, including (Driscoll 2009) and (Gilat 2008). The online documentation is also good.

There are a number of freeware clones of MATLAB available, including Octave and Scilab. These should certainly be adequate for the programs discussed and assigned in this book.

1.1 Desk calculator operations

The basic arithmetic operations in MATLAB use a standard format. The command window can be used as a convenient interactive desk calculator.

```
>> format compact
>> % Comment.  format compact eliminates extra line spaces.
>> x=2+7
x =
```

```
     9

>> y=2*x
y =
    18

>> x+y
ans =
    27

>>% If the user types an expression, the value is assigned to variable "ans"
>> ans^(1/3)
ans =
     3

>> sqrt(2)
ans =
    1.4142

>> format long
>> ans

ans =
   1.414213562373095

>> format short

>> sin(pi/3)
ans =
    0.8660

>> format rat  % display in "rational format", a close rational approximation

>> (1/7)+(1/5)
ans =
      12/35

>> sqrt(2)
ans =
    1393/985
```

1.2 Booleans

MATLAB uses 1 for true and 0 for false. Strictly speaking these are not the same as the integers 1 and 0, but MATLAB automatically casts from one to the other as needed, so the distinction only occasionally makes a difference. (We will see an example in section 2.5.)

```
>> a=5==5
a =
     1
```

```
>> b=5==6
b =
     0

>> a&b
ans =
     0

>> a|b
ans =
     1

>> ~a
ans =
     0

>> a+a %Casting from Boolean to integer
ans =
     2

>> (2-1)&a  %Casting from integer to Boolean
ans =
     1

>> a==2-1
ans =
     1
```

1.3 Non-standard numbers

MATLAB conforms to the IEEE standard for floating point arithmetic (see Overton, 2001), which mandates that a system of floating point arithmetic support the three non-standard values `Inf` (positive infinity), `-Inf` (negative infinity), and `NaN` (Not a Number). These are considered numbers in MATLAB. The infinite values can generally be used numerically in any context where an infinite value makes sense; there are some examples below. `NaN` is used for values that are completely undefined, such as `0/0` or `0*Inf`. Any computation involving `NaN` gives `NaN`; any comparison involving `NaN` is considered false.

```
>> 1/0
ans =
   Inf

>> Inf+Inf
ans =
   Inf

>> Inf*-3
ans =
  -Inf
```

```
>> Inf^2
ans =
   Inf

>> 5 < Inf
ans =
     1

>> 0/0
ans =
   NaN


>> 5 < NaN
ans =
     0

>> 5 >= NaN
ans =
     0

>> sin(Inf)
ans =
   NaN

>> atan(Inf)
ans =
    1.5708
```

1.4 Loops and conditionals

MATLAB has the usual conditional and looping constructs to build complex statements out of simple ones. Note that

- Loops and conditionals end with the key word `end`. Therefore, there is no need for "begin ... end" or "{ ... }" blocks.
- Atomic statements are separated by line breaks. Once a compound statement has been entered, the interpreter continues to read input until the compound statement is ended.
- The value of each atomic statement is printed out as it is executed. This is helpful in debugging; you can trace the execution of a statement just by deleting the semi-colon at the end. To suppress print-out, put a semi-colon at the end.

```
>> for n=1:5
s=s+n
end  % End of user input

s =
```

```
       1
s =
       3
s =
       6
s =
      10
s =
      15


>> for n=1:3
t=a; % Note suppression of printout
a=b
b=t+b
end

a =
     1
b =
     2
a =
     2
b =
     3
a =
     3
b =
     5

>> % Note: Unlike many programming languages, statements are separated by line
>> % breaks
>> x=1;
>> while x < 50
x=x+x
end
x =
       2
x =
       4
x =
       8
x =
      16
x =
      32
x =
      64

>> % The hailstone procedure
>> x=3;
```

```
x =
       3
>> while (x ~= 1)
     if (mod(x,2)==1)
           x=3*x+1
      else x=x/2
     end
   end

x =
      10
x =
       5
x =
      16
x =
       8
x =
       4
x =
       2
x =
       1
```

1.5 Script file

A script file is a plain text file with MATLAB commands. The file has extension .m. To execute a script file that in the working directory, just enter the name of the file (omitting the ".m") in the command window. The working directory can be changed in the "directory" window.

For instance, here is the file p35.m:

```
% p35.m computes x^35 by repeated squaring followed by multiplication

x2=x*x       % x^2
x4=x2*x2     % x^4
x8=x4*x4     % x^8
x16=x8*x8    % x^16
x32=x16*x16  % x^32
x35=x32*x2*x % x^35
```

And this is how to execute it in the command window:

```
>> x=2
x =
       2

>> p35
x2 =
       4
```

```
x4 =
      16
x8 =
     256
x16 =
   65536
x32 =
4294967296
x35 =
34359738368

>> % Variables defined in a script are visible after the script has executed.
>> x4
x4 =
      16

>> % help prints out the comments at the head of the script file.
>> help p35
  p35.m computes x^35 by repeated squaring followed by multiplication
```

1.6 Functions

The MATLAB code for function named foo is in the file foo.m. To call foo in the command window, just type "foo(...)"; this both loads and executes the code.

The main differences between functions and scripts is that variables in a function, including the input and output parameters, are local to the function. (It is also possible to define and access global variables).

The function declaration has one of the two forms

```
   function  <output variable> =  <function name>(input variables)    or
   function [<output variables>] = <function name>(input variables)
```

For instance, here is the file fib.m:

```
% Recursive, very inefficient, definition of Fibonacci numbers

function x = fib(n)
  if (n==0) x=1;
  elseif (n==1) x=1;
  else x=fib(n-1)+fib(n-2);
  end
end
```

And here is its use in MATLAB:

```
>> fib(5)
ans =
```

```
     8

>> help fib
  Recursive, very inefficient, definition of Fibonacci numbers
```

Functions may return multiple values. For example, here is quadform.m:

```
% quadform(a,b,c) returns the two roots of the quadratic equation
% ax^{2} + bx + c = 0

function [r1,r2] = quadform(a,b,c)
  x=sqrt(b^2 - 4*a*c);
  r1=(-b-x)/(2*a);
  r2=(-b+x)/(2*a);
end

>> [p,q]=quadform(1,0,-1)
p =
    -1
q =
     1
```

Function files can have subfunctions. These are placed in the file after the main function (the one with the same name as the file). Subfunctions can be called only by functions within this same file.

Important note: `i` and `j` are used by MATLAB as predefined symbols for the square root of -1. However, MATLAB does not prevent you from using these as variables and reassigning them. If you are not using complex number in your code, which none of the assignments in this book require, this does not usually lead to trouble, but occasionally can cause confusion. The most common case is that, if your code uses `i` or `j` without initializing them, you do not get an error, as with other variables.

```
% In an environment where the user has not initialized either 'a' or 'i'.
>> a+1
??? Undefined function or variable 'a'.

>> i+1
ans =
   1.0000 + 1.0000i
```

1.7 Variable scope and parameter passing

By default a variable used in a function is local to the function call; that is, if a function calls itself recursively, then the variables in the two instances of the functions are different. Variables declared in the command window are local to the command window.

If a variable is declared global in a number of functions then it is shared between all the calls of those functions. If it is also declared global in the command window, then it is also shared with the command window environment.

Parameters are *always* passed call by value. That is, the formal parameters of a function are local variables; the value of the actual parameter is copied into the formal parameter when the function is called, but not copied back when the function returns.

Here is a toy example. Suppose that we have the two functions t1 and t2 defined in the file t1.m as follows:

```
% t1(x) is a toy example used to illustrate global and local variables

function y = t1(x)
global k m
   p=x;
   x=1;
   k=2;
   m=3;
   t2(x)
   y=[p,x,k,m]
end

function t2(z)
global k
    p=11;
    k=12;
    m=14;
    z=16;
end
```

The variable `k` is a global variable shared between t1 and t2. The variable `m` in t1 is a global variable which will be shared with the command window; it is not shared with t2.

We now execute the following in the command window:

```
>> global m

>> k=100
k =
   100

>> m=200
m =
   200

>> p=300
p =
   300

>> x=400
x =
   400

>> t1(x)
y =
```

```
   400     1    12     3
% This is the execution of the last statement of t1:
     y=[p,x,k,m]
% Note that k has been changed by the execution of t2, because it was
% declared global between t1 and t2; the others are unchanged by the
% execution of t2.

% Now back to the command window
y =
   400     1    12     3

>> [p,x,k,m]
ans =
   300   400   100     3

% Note that m has been changed by the execution of t1, because it was
% declared global between the command window and t1. The others are
% unchanged.
```

The use of call-by-value in MATLAB means that if function `f` has parameter `y` and function `g` executes the statement `f(x)` then the value of `x` in `g` must be copied into the variable `y` in `f` before execution of `f` can begin. If `x` is a large matrix, this can involve a significant overhead. Therefore, the programming style which is encouraged in LISP and other similar languages, using large numbers of small functions, and using recursion for implementing loops, is ill-suited to MATLAB. Loops should generally be implemented, if possible, by using MATLAB operators or library functions, or else using iteration.

Copying also occurs at any assignment statement; if `x` is a large matrix, then executing the statement `y=x` involves copying `x` into `y`. If you are executing a long loop involving large arrays, and you are concerned with efficiency, it may be worth giving thought to reducing the number of unnecessary copies.

The truth is that, if your program is largely executing your own MATLAB code (rather than the built-in MATLAB functions, which are implemented efficiently), if it manipulates large quantities of data, and if efficiency is a concern, then you should probably be using some other programming language. Or at least you should write the critical sections of the program in another language; MATLAB has facilities for interfacing with code written in C or C++.

Problem

Problem 1.1

Can you write in MATLAB a function "swap(A,B)" that swaps the values of its arguments? That is, the function should have the following behavior

```
>> i=1;
>> j=5;
>> k=10;

>> swap(i,j);
>> i
```

```
i =
   5
>> j
j =
   1

>> swap(j,k);
>> j
j =
   10
>> k
k =
    1
```

Explain your answer.

Programming Assignments

Note: Since we have not yet defined any data structures, the programming assignments for this chapter are necessarily very numerical in flavor.

Assignment 1.1

A pair of *twin primes* is a pair of prime numbers that differ by two. For example, $\langle 3, 5\rangle$, $\langle 5, 7\rangle$ $\langle 11, 13\rangle$ $\langle 17, 19\rangle$ $\langle 29, 31\rangle$ are the first five pairs of twin primes. It has been conjectured that for large N, the number of twin prime pairs less than N is approximately the function $f(N) = 1.3203 \cdot N/(\log_e N)^2$.

Write a MATLAB function `CountTwinPrimes(N)` that counts the number of twin prime pairs less than `N` and compares the result to the above estimate. That is, your function should return two values

- C, the number of twin-prime pairs less than N
- $|(C - f(N))/f(N)|$, where $f(N)$ is the expression defined above.

You may use the built-in MATLAB function `isprime(X)`.

Assignment 1.2

Goldbach's conjecture asserts that every even number greater than 2 is the sum of two primes. For instance 4=2+2; 6=3+3; 8=3+5; 132=23+109; and so on.

Write a function `Goldbach(N)` which takes as argument an even number N and returns a pair of primes `P,Q` such that `N=P+Q`.

Assignment 1.3

The *four squares* theorem states that every integer can be written as the sum of four square integers. For example

$26 = 5^2 + 1^2 + 0^2 + 0^2$.
$56 = 6^2 + 4^2 + 2^2 + 0^2$.
$71 = 7^2 + 3^2 + 3^2 + 2^2$.

Write a MATLAB function `FourSquaresN` that returns four integers `A,B,C,D` such that `N` = $\texttt{A}^2 + \texttt{B}^2 + \texttt{C}^2 + \texttt{D}^2$.

Assignment 1.4

Write a MATLAB function `TriangleArea(A,B,C)` that computes the area of a triangle with sides of lengths `A,B` and `C`. For instance `TriangleArea(3,4,5)` should return 6. `TriangleArea(1,1,1)` should return 0.4330 ($= \sqrt{3}/4$). `TriangleArea(1,1,sqrt(2)` should return 0.5.

Hint: Look up "Heron's formula" in Wikipedia or your favorite search engine.

Assignment 1.5

The recurrence equation $x_{n+1} = 2x_n^2 - 1$ exhibits *chaotic* behavior for x between -1 and 1. That is, if you compute the series starting from a particular starting point y_0 and then recompute the series starting from a starting point $z_0 = y_0 + \epsilon$ which is very close, the two series grow apart very quickly, and soon the values in one are entirely unrelated to the values in the other.

For example, the two series starting at $y_0 = 0.75$ and $z_0 = 0.76$ are
$y_0 = 0.75$, $y_1 = 0.125$, $y_2 = -0.9688$, $y_3 = 0.8770$, $y_4 = 0.5381$, $y_5 = -0.4209$, $y_6 = -0.6457$.
$z_0 = 0.76$, $z_1 = 0.1552$, $z_2 = -0.9518$, $z_3 = 0.8119$, $z_4 = 0.3185$, $z_5 = -0.7971$, $z_6 = 0.2707$

A. Write a MATLAB function `CompareChaotic(Y0,Z0)` which takes as arguments two starting values y_0 and z_0 and returns the minimum value of n for which $|y_n - z_n| > 0.5$. For instance `CompareChaotic(0.75,0.76)` should return 6, since in the above series $|y_6 - z_6| = 0.9164 > 0.5$.

B. Experiment with a sequence of pairs that are increasingly close together; e.g. $\langle$`Y0` $= .75,$ `Z0` $=$ `0.751`$\rangle, \langle$`Y0` $= 0.75,$ `Z0` $= 0.7501\rangle, \langle$`Y0` $= 0.75,$ `Z0` $= 0.75001\rangle$ and so on. Formulate a conjecture as to how the value of `CompareChaotic(Y0,Z0)` increases with the value of `1/|Y0 - Z0|`.

C. Double precision numbers are represented with about 16 digits (51 bits) of precision. Suppose that you start with a value of y_0 in double precision and compute the series $y_0, y_1, y_2 \ldots$. Given your conjecture in (B), how many terms of the series can you compute before the values become completely unrelated to the true value?

Part I

Linear Algebra

Chapter 2

Vectors

Linear algebra is the study of vectors, discussed in this chapter, and matrices, discussed in chapter 3.

2.1 Definition of vectors

An *n-dimensional vector* is a n-tuple of numbers. (A more general definition will be discussed in section 4.17.) The indices $1 \dots n$ are the *dimensions* of the vector. The values of the tuple are the *components* of the vector.

In this text, we use angle brackets $\langle \dots \rangle$ to delimit vectors.
We will use a letter with an arrow over it, such as $\vec{v}$, to denote a vector. The ith component of vector $\vec{v}$ will be notated $\vec{v}[i]$. (In mathematical writings, it is often notated $\vec{v}_i$, but we will use the subscript exclusively for naming different vectors.)

Example:
$\vec{v} = \langle 0, 6, -2.5 \rangle$ is a 3-dimensional vector. $\vec{v}[1] = 0$. $\vec{v}[3] = -2.5$.

A *zero vector*, denoted $\vec{0}$, is a vector whose components are all 0. E.g. the four-dimensional zero-vector is $\langle 0, 0, 0, 0 \rangle$. (The dimension associated with the notation $\vec{0}$ is determined by context.)

The *unit vector in the i dimension*, denoted $\vec{e}^{\,i}$, is the vector with a 1 in the ith coordinate and 0's everywhere else. For instance, in 4 dimensions, $\vec{e}^{\,2} = \langle 0, 1, 0, 0 \rangle$. The n-dimensional one vector, denoted $\vec{1}$, is the vector with 1's in each dimension; for instance, in 4 dimensions, $\vec{1} = \langle 1, 1, 1, 1 \rangle$.

The set of all n-dimensional vectors is the *n-dimensional Euclidean vector space,* denote $\mathbb{R}^n$.

2.2 Applications of vectors

Vectors can be used in many different kinds of applications. Let us discuss a few typical examples; we will see many more examples in the course of this book.

Application 1: Geometric points

In 2-dimensional geometry, fix a coordinate system $\mathcal{C}$ by specifying an origin, an x-axis, and a y-axis. A point $\mathbf{p}$ can then represented using the vector $\vec{p} = \langle \mathbf{p}[x], \mathbf{p}[y] \rangle$ where $\mathbf{p}[x], \mathbf{p}[y]$ are the coordinates

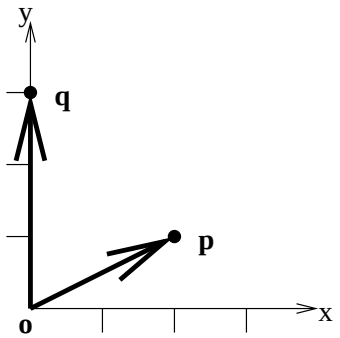


Figure 2.1: Points represented as vectors

of $\mathbf{p}$ in the x and y dimensions. The vector $\vec{p}$ is called the *coordinate vector* for point $\mathbf{p}$, relative to the coordinate system $\mathcal{C}$. For instance in figure 2.1, $\mathbf{p}$ is associated with the vector $\langle 2, 1\rangle$ and $\mathbf{q}$ is associated with the vector $\langle 0, 3\rangle$.

Likewise, in 3-dimensional geometry, point $\mathbf{p}$ can be associated with the vector $\langle \mathbf{p}[x], \mathbf{p}[y], \mathbf{p}[z]\rangle$ of components in the x, y, z dimensions relative to a particular coordinate system. In n-dimensional geometry, point $\mathbf{p}$ can be associated with the vector $\langle \mathbf{p}[1] \ldots \mathbf{p}[n]\rangle$ where $\mathbf{p}[i]$ is the component along the ith coordinate axis.

Geometric coordinates will be discussed at length in chapter 6

Application 2: Time series

A vector can be used to represent a sequence of numeric values of some quantity over time. For instance, the daily closing value of the S&P 500 index over a particular week might be $\langle 900.1, 905.2, 903.7, 904.8, 905.5\rangle$. A patient's hourly body temperature in degrees Farenheit, over a four hour period might be $\langle 103.1, 102.8, 102.0, 100.9\rangle$. Here the dimensions correspond to points in time; the components are the values of the quantity.

Application 3: Almanac information

Numerical information about the fifty states could be recorded in 50-dimensional vectors, where the dimensions corresponds to the states in alphabetical order: Alabama, Alaska, Arizona, Arkansas etc. We could then have a vector
$\vec{p} = \langle 4530000, 650000, 5740000, 2750000 \ldots\rangle$ representing the populations of the states;
$\vec{a} = \langle 52400, 663200, 114000, 2750000 \ldots\rangle$ representing the areas of the states in square miles; and so on.

Application 4: Shopping

The dimensions correspond to a sequence of grocery products: gallon of milk, loaf of bread, apple, carrot, and so on. Each store has a *price vector*; $\vec{s}[i]$ is the price of the ith product at the Stop and Shop; and $\vec{g}[i]$ is the price of the ith product at Gristedes; Each customer has a *shopping list vector*; e.g. a vector $\vec{a}$ where $\vec{a}[i]$ is the number of item i on Amy's shopping list, and $\vec{b}[i]$ is the number of item i on Bob's shopping list; and so on.

Note that, if the dimensions include all products standardly sold in grocery stores, then each shopping list vector is mostly zero. A vector which is mostly zero is called a *sparse* vector; these are common in many applications.

You may well ask, "How should we represent the price of an item that Stop and Shop does not sell?" These are known as null values. In MATLAB, you can use the special value "NaN" (not a number) to represent null values. In programming languages that do not support "NaN", you either have to use a value that is known to be not the price of any actual groceries, such as a negative value or a very large value, or you have a second vector of 1's and 0's that indicates whether or not the object is sold. In either case, applications that use these vectors have to be aware of this representation and take it into account. In fact, in some applications it may be necessary to have more than one kind of null value; for instance, to distinguish items that Stop and Shop does not sell from items where the price is unknown. We will ignore all these issues here and assume that every store has a price for every item.

Application 5: Personal database

Consider a database of personal information for various kinds of applications, such as medical diagnosis, mortgage evaluation, security screening and so on. Each dimension is the result of a numerical measurement or test. Each person has a corresponding vector. The value $\vec{p}[i]$ is the ith feature of person $\vec{p}$. In medical applications you might have age, height, weight, body temperature, various kinds of blood tests, and so on. In financial applications you might have net worth, income, credit score, and so on. (Note that features that are critical in one application may be illegal to use in another.)

Alternatively, one can have a vector for each feature, indexed by person. For instance $\vec{a}$ could be the vector of ages, where $\vec{a}[i]$ is the age of person i.

Application 6: Document analysis

In a library of documents, have one dimension corresponding to each word that appears in any document in the collection. Have a vector for each document in the collection. For document $\vec{d}$ and word w, one can define a vector $\vec{d}$ for each document, where $\vec{d}[w]$ is the number of times word w appears in document d.

Alternatively one can have the dimensions correspond to documents and the vectors correspond to words. That is, for each word w in the collection there is a vector $\vec{w}$. The value of $\vec{w}[d]$ is the number of times word w appears in document d. Both document vectors and word vectors are mostly sparse in most collections.

This use of document vectors was introduced in information retrieval by Gerard Salton (1971). In actual information retrieval systems, the definition of document vector is a little more complex, and gives different weights to different words depending on their frequency; more common words are considered less important. Specifically, let N be the number of documents in a given collection. For any word w, let m_w be the number of documents in the collection that contain w, and let $i_w = \log(N/m_w)$, called the *inverse document frequency*. Note that the fewer documents contain w, the larger i_w; for common words like "the" which are found in all documents, $i_w = 0$. For any document d, let $t_{w,d}$ be the number of occurences of word w in document d. Then we define the document vector $\vec{d}$, indexed by words, so that $\vec{d}[w] = t_{w,d} i_w$.

2.2.1 General comments about applications

Broadly speaking, the above applications come in three categories: geometric interpretations (application 1), sequential interpretations (application 2), and numeric functions of two entities/features (applications 3-6). We will see some other categories, but these three categories include many of the applications of vectors. A couple of general points may be noted.

First, the geometric interpretations depend on an arbitrary choice of coordinate system: how a *point* is modelled as a *vector* depends the choice of the origin and x- and y-axes. It will therefore be an important question how different choices of coordinate system affect the association of vectors with points. In other categories, there is generally a natural coordinate system and the only similar arbitrary choice is the choice of unit (e.g. feet rather than meters; US dollars rather than euros; liters instead of gallons; etc.) Even in those cases, as we shall see at length in chapter 7, it is often important to think about alternative, less natural, coordinate systems.

Second, in the first and third categories, the association of dimensions with numerical indices is essentially arbitrary. There is no particular reason that the states should be listed in alphabetical order; they could just as well be listed in backward alphabetical order (Wyoming, West Virginia, Washington ...), in order of admission to the union (Delaware, Pennsylvania, New Jersey ...), or any other order. Any question whose answer depends on having a particular order, such as "Are there three consecutive states with populations greater than 7 million?" is almost certain to be meaningless. Likewise, in geometric applications, there is no particular reason that the x, y, and z direction are enumerated in that order; the order z, x, y is just as good.[1] In time series and other sequential vectors, by contrast, the numeric value of the index is significant; it represents the time of the measurement.

In a programming language such as Ada that supports enumerated types and arrays that are indexed on enumerated types, the programmer can declare explicitly that, for instance, the vectors in application 3 are indexed on states or that the person vectors in application 5 are indexed on a specified list of features. However, MATLAB does not support the type structure needed for this. For the vectors of application 4 indexed by product type, or the vectors of application 6 indexed by document or words, where the class of indices is not predetermined, one would want arrays indexed on *open* types, such as words; I don't know of any programming language that supports this.

This distinction is not reflected in standard mathematical notations; mathematicians, by and large, are not interested in issues of types in the programming language sense.

2.3 Basic operations on vectors

There are two basic[2] operations on n-dimensional vectors:

- Multiplying a n-dimensional vector by a number. This is done component by component and the result is a new n-dimensional vector. That is, if $\vec{w} = r \cdot \vec{v}$ then $\vec{w}[i] = r \cdot \vec{v}[i]$.

  E.g. $4 \cdot \langle 3, 1, 10 \rangle = \langle 4 \cdot 3,\ 4 \cdot 1,\ 4 \cdot 10 \rangle = \langle 12, 4, 40 \rangle$.

[1] There is, however, a significant distinction between left- and right-handed coordinate systems, which is related to the order of the coordinates; see section 7.1.2.

[2] "Sez who?" you may well ask. What's so not basic about operations like finding the length of a vector, adding a scalar to a vector, finding the largest element of a vector, or sorting a vector? Certainly these are important and of course they are built into MATLAB. There are, however, two related reasons for emphasizing these two operations. First, as we shall see, linear algebra is essentially about linear transformations; the two operations of vector addition and scalar multiplication are linear transformations while operations like sorting are not. Second, in the more general definition of vector discussed in section 4.17, these other operations may not be pertinent. For instance the components of a vector may be entities that are not ordered in terms of "greater" and "less". In that case sorting is not meaningful.

In linear algebra, a number is often called a *scalar*, so multiplication by a number is called *scalar multiplication.*

It is conventional to write $a \cdot \vec{v}$ rather than $\vec{v} \cdot a$. The value $(-1) \cdot \vec{v}$ is written $-\vec{v}$. As usual in mathematical notation, we may omit the multiplicative dot symbol and just write $a\vec{v}$ when that is not confusing.

- Adding two vectors of the same dimension. This is done component by component; that is, if $\vec{w} = \vec{v} + \vec{u}$ then $\vec{w}[i] = \vec{v}[i] + \vec{u}[i]$.
  E.g. $\langle 3, 1, 10\rangle + \langle 1, 4, -2\rangle = \langle 3+1,\ 1+4,\ 10-2\rangle = \langle 3, 5, 8\rangle$.

  Two vectors of different dimensions may not be added.

  The difference of two vectors $\vec{v} - \vec{u}$ is defined as $\vec{v} + (-\vec{u})$.

2.3.1 Algebraic properties of the operations

The following basic properties of these operators are important. They are all easily proven from the definitions.

In all the following, $\vec{v}$, $\vec{u}$, $\vec{w}$ and $\vec{0}$ are n-dimensional vectors and a and b are numbers.

$\vec{v} + \vec{u} = \vec{u} + \vec{v}$. (Commutativity)
$(\vec{v} + \vec{u}) + \vec{w} = \vec{v} + (\vec{u} + \vec{w})$. (Associativity).
$a \cdot (\vec{v} + \vec{u}) = (a \cdot \vec{v}) + (a \cdot \vec{u})$. (Distributivity).
$(a + b) \cdot \vec{v} = (a \cdot \vec{v}) + (b \cdot \vec{v})$ (Distributivity).
$a \cdot (b \cdot \vec{v}) = (ab) \cdot \vec{v}$.
$0 \cdot \vec{v} = \vec{0}$.
$\vec{v} + \vec{0} = \vec{v}$. ($\vec{0}$ is the additive identity).
$\vec{v} - \vec{v} = \vec{0}$. ($-\vec{v}$ is the additive inverse).

2.3.2 Applications of basic operations

Geometric. Fix a coordinate system in space with origin **o**. Suppose that $\vec{p}$ and $\vec{q}$ are the coordinate vectors for points **p** and **q**. Let a be a number. Draw arrows from **o** to **p** and **q** respectively

If you take the arrow from **o** to **p**, make it a times as long, keeping the direction the same and the tail of the arrow at **o**, then the coordinate vector of the head of the arrow is $a\vec{p}$.

If you copy the arrow from **o** to **q**, keeping the direction and length the same, and put its tail at **p**, then the coordinate vector of the head of the arrow is $\vec{p} + \vec{q}$.

Figure 2.2 illustrates this with $\vec{p} = \langle 2, 1\rangle$, $\vec{q} = \langle 0, 3\rangle$, $\alpha = 1.5$.

Non-geometric: The non-geometric interpretations of vector addition and scalar multiplication are mostly obvious. You multiply by a scalar when you need to multiply every component; you add two vectors when you need to add every component. For example, consider example 4 above, where the dimensions correspond to different kind of groceries. If $\vec{a}$ is Amy's shopping list, and $\vec{b}$ is Bob's, and they decide to shop together, then $\vec{a} + \vec{b}$ is their joint shopping list. If $\vec{s}$ is the price list for Stop and Shop and $\vec{g}$ is the price for Gristede's then $\vec{v} - \vec{g}$ is the amount you save at Gristede's for each item. (If negative, then the item is more expensive at Gristede's). If Shop and Shop announces a 20% off sale on all items in the store, then the new price vector is $0.8 \cdot \vec{s}$. If you want to convert a price vector from dollars to euros, you multiply by the current exchange rate. Other applications work similarly.

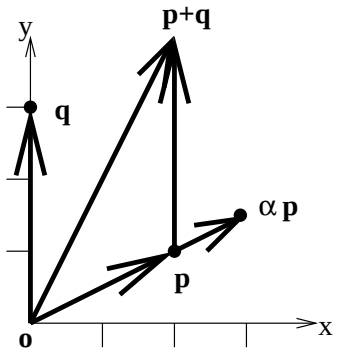


Figure 2.2: Points represented as vectors

2.4 Dot product

The *dot product* of two n-dimensional vectors is computed by multiplying corresponding components, and then adding all these products. That is,

$$\vec{v} \bullet \vec{w} = \vec{v}[1] \cdot \vec{w}[1] + \ldots + \vec{v}[n] \cdot \vec{w}[n]$$

For example, $\langle 3, 1, 10 \rangle \bullet \langle -2, 0, 4 \rangle = (3 \cdot -2) + (1 \cdot 0) + (10 \cdot 4) = -6 + 0 + 40 = 34$

The dot product is also known as the *scalar product* or the *inner product*. We will use a large solid dot $\bullet$ as above; this is not standard mathematical notation, but otherwise a long sequence of small dots can be confusing.

The dot product is not defined for vectors of different dimensions.

2.4.1 Algebraic properties of the dot product

The following basic properties of the dot product are important. They are all easily proven from the above definition. In the following, $\vec{v}$, $\vec{u}$ and $\vec{w}$ are n-dimensional vectors and a is a number.

$\vec{v} \bullet \vec{u} = \vec{u} \bullet \vec{v}$. (Commutative)
$(\vec{u} + \vec{v}) \bullet \vec{w} = (\vec{u} \bullet \vec{w}) + (\vec{v} \bullet \vec{w})$. (Distributive)
$(a \cdot \vec{u}) \bullet \vec{v} = a \cdot (\vec{u} \bullet \vec{v}) = \vec{u} \bullet (a \cdot \vec{v})$

Another obvious but important property is that the dot product of vector $\vec{v}$ with the i-th unit vector $\vec{e}^{\,i}$ is equal to i-th coordinate $\vec{v}[i]$. We will see a generalization of this in section 4.3.

2.4.2 Application of the dot product: Weighted sum

The simplest applications of the dot product are to compute weighted sums. A few examples:

In the grocery shopping application (application 4 above), let $\vec{s}$ be the vector of prices at Stop and Shop, and let $\vec{a}$ be Amy's shopping list. Then, if Amy goes shopping at Stop and Shop, she will pay $\vec{a}[i] \cdot \vec{s}[i]$ for the item i, and therefore her total bill will be $\sum_i \vec{a}[i] \cdot \vec{s}[i] = \vec{a} \bullet \vec{s}$.

The sum of the elements of an n-dimensional vector $\vec{v}$ is $\vec{1} \cdot \vec{v}$. The average value of a n-dimensional vector $\vec{v}$ is the sum divided by n, thus $(1/n) \cdot \vec{1} \bullet \vec{v}$.

In the almanac application (application 3) let $\vec{p}$ be the population of each state and let $\vec{q}$ be the average income in each state. Then $\vec{p}[i] \cdot \vec{q}[i]$ is the total income of all people in state i, so $\vec{p} \bullet \vec{q}$ is the total income of everyone in the country. The average income across the country is the total income divided by the population, $(\vec{p} \bullet \vec{q})/(\vec{p} \bullet \vec{1})$. Note that you are not allowed to "cancel out" the $\vec{p}$ in the numerator and denominator; dot product doesn't work that way.

Application 7: Linear classifiers. An important category of applications are *classification* problem. You are given a description of an entity in terms of a vector $\vec{v}$ of some kind, and you want to know whether the entity belongs to some specific category. For instance, a bank has collected information about a loan applicant, and wants to decide whether he/she is a reasonable risk. A doctor has a collection of information (symptoms, medical history, test results . . .) about a patient, and wants to know whether the patient suffers from a particular disease. A spam filter has the text of an email message, encoded as a document vector (see application 6 above) and wants to know whether the message is spam.

A *classifier* for the category is an algorithm that takes the vector of features as input and tries to calculate whether the entity is or is not an instance of the category. One of the simplest and most widely used kind of classifier is a *linear classifier*, which consists of a vector of weights $\vec{w}$ and a threshhold t. If the weighted sum of the feature vector, $\vec{w} \bullet \vec{v} > t$, then the classifier predicts that the entities is in the category; otherwise, the classifier predicts that it is not.

Most machine learning programs work by constructing a classifier for a category, based on a corpus of examples. One simple algorithm to do this, the *Naive Bayes* algorithm, will be discussed in section 8.11.

2.4.3 Geometric properties of the dot product

Geometrical analysis yields further interesting properties of the dot product operation that can then be used in non-geometric applications. This takes a little work.

Consider a fixed two-dimensional coordinate system with origin **o**, an x-axis and a y-axis. Let **p** and **q** be points and let $\vec{p}$ and $\vec{q}$ be the associated coordinate vectors.

First, note that, by the Pythagorean theorem, the distance from **o** to **p** (in the units of the coordinate system), which we will denote $d(\mathbf{o}, \mathbf{p})$ is

$$\sqrt{\vec{p}[x]^2 + \vec{p}[y]^2}$$

But $\vec{p}[x]^2 + \vec{p}[y]^2 = \vec{p} \bullet \vec{p}$. So $d(\mathbf{o}, \mathbf{p}) = \sqrt{\vec{p} \bullet \vec{p}}$. This quantity $\sqrt{\vec{p} \bullet \vec{p}}$ is called the *length* of vector $\vec{p}$ and is denoted $|\vec{p}|$.

Similarly,

$$d(\mathbf{p}, \mathbf{q}) = \sqrt{(\vec{q}[x] - \vec{p}[x])^2 + (\vec{q}[y] - \vec{p}[y])^2}$$

So

$$d(\mathbf{p}, \mathbf{q})^2 = (\vec{q}[x] - \vec{p}[x])^2 + (\vec{q}[y] - \vec{p}[y])^2 = (\vec{q} - \vec{p}) \bullet (\vec{q} - \vec{p}) = \vec{q} \bullet \vec{q} - 2\vec{p} \bullet \vec{q} + \vec{p} \bullet \vec{p} = d(\mathbf{o}, \mathbf{q})^2 - 2\vec{p} \bullet \vec{q} + d(\mathbf{o}, \mathbf{p})^2$$

Therefore

$$\vec{p} \bullet \vec{q} = \frac{d(\mathbf{o}, \mathbf{p})^2 + d(\mathbf{o}, \mathbf{q})^2 - d(\mathbf{p}, \mathbf{q})^2}{2} \tag{2.1}$$

We have proven this for two-dimensional points, but in fact the same proof works in Euclidean space of any dimension.

Proceeding from the above formula, a number of important conclusions can be deduced. First, we know by the triangle inequality that

$$|d(\mathbf{o}, \mathbf{p}) - d(\mathbf{o}, \mathbf{q})| \leq d(\mathbf{p}, \mathbf{q}) \leq d(\mathbf{o}, \mathbf{p}) + d(\mathbf{o}, \mathbf{q})$$

Since all these are non-negative, we may square all parts of the inequality, giving

$$d(\mathbf{o},\mathbf{p})^2 - 2d(\mathbf{o},\mathbf{p})d(\mathbf{o},\mathbf{q}) + d(\mathbf{o},\mathbf{q})^2 \leq d(\mathbf{p},\mathbf{q})^2 \leq d(\mathbf{o},\mathbf{p})^2 + 2d(\mathbf{o},\mathbf{p})d(\mathbf{o},\mathbf{q}) + d(\mathbf{o},\mathbf{q})^2$$

Therefore

$$-2d(\mathbf{o},\mathbf{p})d(\mathbf{o},\mathbf{q}) \leq d(\mathbf{o},\mathbf{p})^2 + d(\mathbf{o},\mathbf{q})^2 - d(\mathbf{p},\mathbf{q})^2 \leq 2d(\mathbf{o},\mathbf{p})d(\mathbf{o},\mathbf{q})$$

But by equation 2.1 the middle term here is just $2\vec{p} \bullet \vec{q}$. Substituting and dividing through by 2 gives

$$-d(\mathbf{o},\mathbf{p})d(\mathbf{o},\mathbf{q}) \leq \vec{p} \bullet \vec{q} \leq d(\mathbf{o},\mathbf{p})d(\mathbf{o},\mathbf{q})$$

Using the facts that $d(\mathbf{o},\mathbf{p}) = |\vec{p}|$ and $d(\mathbf{o},\mathbf{q}) = |\vec{q}|$, and dividing through gives

$$-1 \leq \frac{\vec{p} \bullet \vec{q}}{|\vec{p}| \cdot |\vec{q}|} \leq 1 \tag{2.2}$$

Equation 2.2 is known as the *Cauchy-Schwarz inequality.*[3]

Second, consider the case where $\mathbf{p}, \mathbf{o}, \mathbf{q}$ form a right angle; that is, the arrow from $\mathbf{o}$ to $\mathbf{q}$ is at right angles to the arrow from $\mathbf{o}$ to $\mathbf{p}$. Then by the Pythagorean theorem, $d(\mathbf{p},\mathbf{q})^2 = d(\mathbf{o},\mathbf{p})^2 + d(\mathbf{o},\mathbf{q})^2$. Using equation 2.1 it follows that $\vec{p} \bullet \vec{q} = 0$. In this case, we say that $\vec{p}$ and $\vec{q}$ are *orthogonal.*

Equation 2.2 can be made more precise. Let θ be the angle between the arrow from $\mathbf{o}$ to $\mathbf{q}$ and the arrow from $\mathbf{o}$ to $\mathbf{p}$. Recalling the law of cosines from trigonometry class in the distant past and applying it to the triangle $\mathbf{opq}$, we have

$$d(\mathbf{p},\mathbf{q})^2 = d(\mathbf{o},\mathbf{p})^2 + d(\mathbf{o},\mathbf{q})^2 - 2d(\mathbf{o},\mathbf{p})d(\mathbf{o},\mathbf{q})\cos(\theta)$$

so

$$\cos(\theta) = \frac{d(\mathbf{o},\mathbf{p})^2 + d(\mathbf{o},\mathbf{q})^2 - d(\mathbf{p},\mathbf{q})^2}{2d(\mathbf{o},\mathbf{p})d(\mathbf{o},\mathbf{q})} = \frac{\vec{p} \bullet \vec{q}}{|\vec{p}| \cdot |\vec{q}|}$$

Thus, the angle θ between the two vectors $\vec{p}$ and $\vec{q}$ can be calculated as $\cos^{-1}(\vec{p} \bullet \vec{q}/|\vec{p}||\vec{q}|)$.

Another way to write this formula is using *unit vectors.* A unit vector is a vector of length 1. For any vector $\vec{v} \neq \vec{0}$, the unit vector in the same direction as $\vec{v}$ is just $\vec{v}/|\vec{v}|$; this is often written $\hat{v}$. So we can rewrite the above formula

$$\cos(\theta) = \frac{\vec{p}}{|\vec{p}|} \bullet \frac{\vec{q}}{|\vec{q}|} = \hat{p} \bullet \hat{q} \tag{2.3}$$

We have used this geometric argumentation to derive important properties of the dot product, but we have not said what, in general, the dot product actually *means*, geometrically. Sadly, there is no very intuitive or interesting answer to that. (Equations 2.1 and 2.3 are geometrical definitions but they do not give a clear intuitive sense for the dot product.) The best, perhaps, is this: Given $\vec{p}$ and $\vec{q}$, let $\vec{w}$ be the vector that is perpendicular to $\vec{q}$, in the same plane as $\vec{p}$ and $\vec{q}$, and the same length as $\vec{q}$. Then $|\vec{p} \bullet \vec{q}|$ is the area of the parallelogram with side $\vec{p}$ and $\vec{w}$ (figure 2.3). This is not a very helpful definition, however; first, because the distributivity rule is not geometrically obvious; second, because the sign of the dot product is not easy to define in this way.

[3]This may seem a little suspicious to you: how did we derive this non-trivial algebraic inequality from this simple geometric argument? If it does seem suspicious, then you have good instincts; what we've pushed under the rug here is proving that the triangle inequality holds for Euclidean distance in n-dimensions.

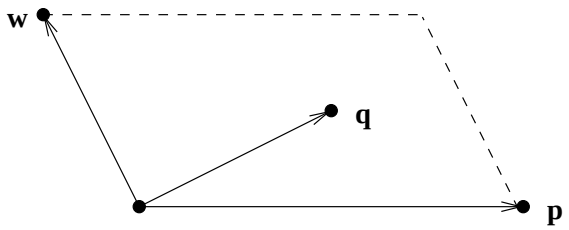


Figure 2.3: Geometric interpretation of the dot product

2.4.4 Metacomment: How to read formula manipulations

The derivation of the Cauchy-Schwarz inequality in the previous section is a sterling example of what people dislike about math and math books: "⟨Dull long formula⟩ so ⟨series of even duller, even longer formulas⟩ so ⟨pretty dull but short formula⟩. Isn't that wonderful!"

I can't eliminate formula manipulation from this book, because that is an important part of how math works. I can't always replace formula manipulation proofs with "insightful" proofs because a lot of the time there aren't any insightful proofs. Moreover, proofs that avoid formula manipulation are not necessarily more insightful. Sometimes they rely on a trick that is actually largely beside the point. Sometimes they don't generalize as well.

The one thing that I can do is to tell you how I read this kind of thing, and I suggest that you do likewise. Trying to read these the way one would read the newspaper, or even the way one would read the earlier sections of this chapter, is for me a complete waste of time. (Of course, people are all different, and there may be someone somewhere who gets something out of that; but no one I've ever met.) I find that there are three possible approaches:

1. The best is to glance through it, get kind of an idea how it works, close the book, and try to write out the proof yourself without looking at the book. Unless the proof is quite short, you should write it out rather than trying to think it through in your head. Once you've done this, you really understand how the proof works and what it means.

2. If you're dealing with a long proof or if you're short on time, (1) will probably be too hard. In that case the second best is to go through it *slowly.* Check the simple steps of the proof by eye, making sure that you keep track of where all the terms go, and that you understand why the author brought in another formula from before at this point. If you can't follow the step by eye, then copy it down and work it out on paper. The limitation of this, as opposed to (1), is that you can end up understanding each of the steps but not the overall progress of the proof; you hear the notes but not the overall tune.

In either (1) or (2), if the book provides a picture/example, then you should carefully look at it and make sure you understand the connection between the picture/example and the proof. If the book doesn't provide one, then you should draw a picture, if the proof is geometric, or you should work through some numeric examples, if the proof is numeric. Manipulating the numbers often gives you a clearer sense of what is going on than looking at the algebraic symbols.

(1) and (2) are both *hard* and *time-consuming*, but there is no way around that if you want to learn the math. "There is no royal road to geometry" (Euclid). That leaves option (3): Skip the manipulation and just learn the conclusion. Unless you are responsible for the manipulation — you are reviewing the proof for a scientific journal, or your instructor has told you that you are required to know the proof for the exam — this is probably safe to do. In my job, I regularly read books and articles with proofs in them; I work through perhaps 5% of them, probably less. Your time is valuable, and there are other things to do in life. But though you can do this sometimes, you can't

always take this approach, if you want to learn how to do math.

2.4.5 Application of the dot product: Similarity of two vectors

The geometric discussion of the previous section can be applied to non-geometric vectors to give two measures of how close or similar two vectors are.

The obvious measure of the similarity between two vectors $\vec{p}$ and $\vec{q}$ is just the distance between them $|\vec{q}-\vec{p}| = \sqrt{(\vec{q}-\vec{p}) \bullet (\vec{q}-\vec{p})}$. For instance, if you have a set of pricing vectors from different stores, as in application 4, and you want to determine which stores have most similar pricing policies (perhaps with a view to detecting price fixing) this might be a reasonable measure to use. Note that if you are just comparing greater and lesser distances, there is no need to extract the square root; we can just use the distance squared, which is equal to $(\vec{q}-\vec{p}) \bullet (\vec{q}-\vec{p})$.

However, it is often more pertinent to consider a *scale invariant* measure of similarity of two vectors, in which one is interested in the difference in the direction of the two vectors independent of their magnitude. In that case, a natural measure is the angle between the two vectors, which can be calculated in terms of the expression $(\vec{p} \bullet \vec{q})/(|\vec{p}| \cdot |\vec{q}|)$. Again, if one is just comparing greater and smaller angles, there is no need to calculate the inverse cosine function to get the actual angle; it suffices just to calculate the cosine of the angle using this formula.

For example, suppose we want to evaluate the similarity of two documents in terms of the words they use – for example, to suggest "related documents" in a search engine. We can then use the document model described in application 6 above. If we just use the distance between the document vectors, then long documents will tend to be close to other long documents and far from short documents, which is not at all what we want. Rather, we want to base the similarity judgement on the relative frequency of words in the documents. This can be done by using the angle cosine between the document vectors.

Application 8: Recommender systems A company wants to recommend specific products to specific user. (Netflix recently sponsored a $1,000,000 competition for the programmer who produced the best program to recommend movies.) The company has available a large database of purchases by customers.

One way to do this, in principle,[4] is the following: For each customer in the data base, construct a vector indexed by product. That is, corresponding to customer c, construct an n-dimensional vector $\vec{c}$ where n is the number of different products, and where $\vec{c}[i]$ is equal to the quantity of product i that customer c has bought. Of course $\vec{c}[i]$ is 0 for most i; thus this is a sparse vector. Now, in making recommendations for customer d, find the k customer vectors that are most similar to $\vec{d}$ in terms of the above measure, and recommend products that have been popular among these customers.

There is also a dual approach: For each product p, construct an m-dimensional vector $\vec{p}$ where m is the number of different customers, and where $\vec{p}[j]$ is the quantity of product p that customer j has bought. To find customers who might like a specific product q, look for the k product vectors most similar to $\vec{q}$, and recommend q to customers who have bought some of these products.

Application 9: Pattern comparison Suppose we want to compare the pattern of the stock market crash of fall 1929 with the stock market crash of fall 2008. Since the Dow Jones average was around 700 at the start of September 1929 and around 12,000 at the start of September 2008, there is no point in using the distance between the corresponding vectors. The angle cosine between the two vectors might be a more reasonable measure.

[4] Getting this method to work efficiently for a huge database is not easy.

Application 10: Statistical correlation.[5] A course instructor wishes to determine how well the results on his final exam correspond to the results on the problem sets. Suppose that there are six students in the class; the vector of average problem set scores was $\vec{p} = \langle 9.1, 6.2, 7.2, 9.9, 8.3, 8.6 \rangle$ and the vector of final exam scores was $\vec{x} = \langle 85, 73, 68, 95, 77, 100 \rangle$.

The first step is to shift each vector so that they are both zero-centered; otherwise, the comparison will mostly just reflect the fact that students as a whole did fairly well on both. We are interested in the performances of individual students relative to the average, so we subtract the average value from each vector. The average problem set score $\bar{p} = 8.22$ and the average exam score $\bar{e} = 83$, so the shifted vectors are $\vec{p}\,' = \vec{p} - \bar{p} \cdot \vec{1} = \langle 0.8833, -2.0167, -1.0167, 1.6833, 0.0833, 0.3833, \rangle$ and $\vec{x}\,' = \vec{x} - \bar{e} \cdot \vec{1} = \langle 2, -10, -15, 12, -6, 17 \rangle$

The correlation is the angle cosine between these, $\vec{p}\,' \bullet \vec{x}\,' / |\vec{p}\,'||\vec{x}\,'| = 0.7536$

In general, the correllation between two vector $\vec{p}$ and $\vec{q}$ is defined by the following algorithm

$\vec{p}\,' \leftarrow \vec{p} - Mean(\vec{p}) \cdot \vec{1}$;
$\vec{q}\,' \leftarrow \vec{q} - Mean(\vec{q}) \cdot \vec{1}$;
$Correlation \leftarrow \vec{p}\,' \bullet \vec{q}\,' / |\vec{p}\,'|\,|\vec{q}\,'|$.

2.4.6 Dot product and linear transformations

The fundamental significance of a dot product is that it is a linear transformation of vectors. This is stated in theorem 2.1 below, which though easily proven is very profound. First we need a definition.

Definition 2.1. *Let $f(\vec{v})$ be a function from n-dimensional vectors to numbers. We say that f is a* linear transformation *if it satisfies the following two properties:*

- *For any vector $\vec{v}$ and scalar a, $f(a \cdot \vec{v}) = a \cdot f(\vec{v})$.*
- *For any vectors $\vec{v}, \vec{u}$, $f(\vec{v} + \vec{u}) = f(\vec{v}) + f(\vec{u})$.*

The algebraic properties of the dot product listed in section2.4.1 show the following: For any vector $\vec{w}$, the function $f(\vec{v}) = \vec{w} \bullet \vec{v}$ is a linear transformation. Theorem 2.1 establishes the converse: Any linear transformation $f(\vec{v})$ corresponds to the dot product with a weight vector $\vec{w}$.

Theorem 2.1. *Let f be a linear transformation from n-dimensional vectors to numbers. Then there exists a unique vector $\vec{w}$, such that, for all $\vec{v}$, $f(\vec{v}) = \vec{w} \bullet \vec{v}$.*

For example, imagine that Stop and Shop does not post the price of individual items; the checkout clerk just tells you the price of an entire basket. Let f be the function that maps a given shopping basket to the total price of that basket. The function f is linear assuming that Stop and Shop has no "two for the price of one" offers, "maximum of one per customer" restrictions etc. Specifically,

1. If you multiply the number of each kind of item in a basket $\vec{b}$ by a, then the total price of the basket increases by a factor of a.
2. If you combine two baskets $\vec{b}$ and $\vec{c}$ into a single basket $\vec{b} + \vec{c}$, then the price of the combined basket is just the sum of the prices of the individual baskets.

Then theorem 2.1 states that there is a price vector $\vec{s}$ such that $f(\vec{b}) = \vec{s} \bullet \vec{b}$ for any basket $\vec{b}$. How do we find the vector $\vec{s}$? Couldn't be simpler. Put a single unit of a single item i into a basket, and

[5] This example is adapted from Steven Leon, *Linear Algebra with Applications.*

ask Stop and Shop the price of that basket. We will call that the "price of item i", and we set $\vec{s}[i]$ to be that price. By property (1), a basket that contains $\vec{b}[i]$ units of item i and nothing else costs $\vec{b}[i] \cdot \vec{s}[i]$. By property (2), a basket that contains $\vec{b}[1]$ units of item 1, $\vec{b}[1]$ units of item 2 ... and $\vec{b}[n]$ units of item n costs $\vec{b}[1] \cdot \vec{s}[1] + \vec{b}[2] \cdot \vec{s}[2] + \ldots \vec{b}[n] \cdot \vec{s}[n] = \vec{s} \bullet \vec{b}$.

The general proof of theorem 2.1 is exactly the same as the argument we have given above for Stop and Shop prices.[6]

2.5 Vectors in MATLAB: Basic operations

In this section we illustrate the basic vector operations and functions by example. For the most part, these examples are self-explanatory; in a few cases, we provide a brief explanation.

Strictly speaking, MATLAB does not have a separate category of vectors as such; vectors are either $1 \times n$ matrices (row vectors) or $n \times 1$ matrices (column vectors). Most functions that take a vector argument, such as `dot`, `norm`, and `plot`, do the same thing with either kind of vector. Functions that return a vector value, such as `size` and `randperm`, have to choose, of course; these mostly return row vectors, presumably because they print out more compactly.

Creating a vector; indexing; setting a component.

```
>> v = [2,3,2,5,11]
v =
     2     3     2     5    11

>> a=v(4)
a =
     5

>> v(4)=8
v =
     2     3     2     8    11

>> v(8)=10
v =
     2     3     2     8    11     0     0    10
% If you set a positive index beyond the range of the vector,  Matlab
% expands the vector to accommodate.

>> v(10)
??? Attempted to access v(10); index out of bounds because numel(v)=5.
% But not if you try to access beyond the range.

>> v(-2)=3
??? Attempted to access v(-2); index must be a positive integer or logical.

% or if you try to set an invalid index.
```

Creating a vector with elements in arithmetic sequence:

[6] The theorem does not hold, however, for infinite-dimensional vector spaces.

```
>> u=2:10
u =
     2     3     4     5     6     7     8     9    10

>> w= 3.16 : 0.5 : 6.0
w =
    3.1600    3.6600    4.1600    4.6600    5.1600    5.6600

>> ones(1,5)
ans =
     1     1     1     1     1

>> zeros(1,5)
ans =
     0     0     0     0     0
```

Boolean vectors

```
>> q=[12,3,1,7,2]
q =
    12     3     1     7     2

>> p=[1,3,5,7,9]
p =
     1     3     5     7     9

>> p==q
ans =
     0     1     0     1     0
```

Subvectors

```
>> w
w =
    3.1600    3.6600    4.1600    4.6600    5.1600    5.6600

>> w(2:4)
ans =
    3.6600    4.1600    4.6600

>> w(1:2:6)
ans =
    3.1600    4.1600    5.1600

>> q
q =
    12     3     1     7     2

>> q([3,3,1,5])
ans =
     1     1    12     2
```

```
>> q(2:4)=[4,1,6]
q =
    12     4     1     6     2

>> q<5
ans =
     0     1     1     0     1

>> q(q<5)
ans =
     4     1     2

>> % However, the following looks like it should be the same but give an error
>> q([0,1,1,0,1])
??? Subscript indices must either be real positive integers or logicals.

>> % Why? Because [0,1,1,0,1], entered from the keyboard, is a vector of
>> % integers, not a vector of Booleans, and Matlab can't figure out that it
>> % needs to do a cast.  So you have to do an explicit cast.

>> q(logical([0,1,1,0,1]))
ans =
     4     1     2

>> % This is why a programming language should not have two basic constants
>> % (numeric 0 vs. logical 0) that print in the same way.
```

Basic operations:

```
>> u
u =
     2     3     4     5     6     7     8     9    10

>> 3*u
ans =
     6     9    12    15    18    21    24    27    30

>> 3+u
ans =
     5     6     7     8     9    10    11    12    13

>> u+(6:14)
ans =
     8    10    12    14    16    18    20    22    24

>> u+w
??? Error using ==> plus
Matrix dimensions must agree.
```

Element by element operations: In MATLAB, the notation `u * v` means matrix multiplication (to be discussed in chapter 3). Therefore, if we want to multiply two vectors element by element,

we use special notation `u .* v` (period asterisk). Likewise with some other operations, such as exponentiation, that have a particular meaning for matrices, one uses a leading dot to signify an element-by-element operation.

```
>> u
u =
     2     3     4     5     6     7     8     9    10

>> u.*(u+3)
ans =
    10    18    28    40    54    70    88   108   130

>> u./(u+3)
ans =
  Columns 1 through 7
    0.4000    0.5000    0.5714    0.6250    0.6667    0.7000    0.7273
  Columns 8 through 9
    0.7500    0.7692

>> u.^2
ans =
     4     9    16    25    36    49    64    81   100

>> % Numerical functions with no particular matrix significance
>> %can be applied without using the . notation
>> sin(u)
ans =
  Columns 1 through 7
    0.9093    0.1411   -0.7568   -0.9589   -0.2794    0.6570    0.9894
  Columns 8 through 9
    0.4121   -0.5440
```

Useful vector functions:

```
>> u
u =
     2     3     4     5     6     7     8     9    10

>> mean(u)
ans =
     6

>> length(u) % Number of dimensions
ans =
     9

>> norm([3,4]) % Euclidean length
ans =
     5

>> norm(u)
```

```
ans =
   19.5959

>> ans^2
ans =
  384.0000

>> max(u)
ans =
    10

>> min(u)
ans =
     2

>> sum(u)
ans =
    54

>> sort([5,2,1,6,1,8])
ans =
     1     1     2     5     6     8

>> median([5,2,1,6,1,8])
ans =
    3.5000

>> dot([1,2,3],[3,2,1])
ans =
    10
```

Random vector:

```
>> rand(1,5) % 1,5 because this is a random 1x5 matrix.
ans =
    0.8147    0.9058    0.1270    0.9134    0.6324

>> randperm(8) % random permutation of 1:8
ans =
     1     6     2     3     8     4     5     7
```

Example: Correlation

Calculation of the correlation of exam scores and problem sets

```
>> function cor = correlation(u,v)
     uprime = u - mean(u);
     vprime = v - mean(v);
     cor = dot(uprime/norm(uprime), vprime/norm(vprime));
   end

>> e=[85, 73, 68, 95, 77, 100]
```

```
e =
    85    73    68    95    77   100

>> p= [ 9.1, 6.2, 7.2, 9.9, 8.3, 8.6 ]
p =
    9.1000    6.2000    7.2000    9.9000    8.3000    8.6000

>> correlation(e,p)
ans =
    0.7536
```

Strings: Vectors of characters

```
>> s='Call me Ishmael'
s =
Call me Ishmael

>> s(5:10)
ans =
 me Is
```

Sparse vectors. To create a sparse vector with all 0's of length n, call `sparse(1,n)`. (Again, the argument "1" is because this is a $1 \times$ n matrix.) To turn an ordinary (full) vector v into a sparse vector s, call `s=sparse(v)`; to go the other way, call `v=full(s)`. Indexing, vector addition, scalar multiplication, and most vector functions work with sparse vectors exactly or nearly the same way as with full vectors.

```
>> v=sparse(1,10) % 1,10 because this is a sparse 1x10 matrix.
v =
   All zero sparse: 1-by-10

>> full(v)
ans =
     0     0     0     0     0     0     0     0     0     0

>> v(2)=3
v =
   (1,2)        3

>> u=sparse(1,10)
u =
   All zero sparse: 1-by-10

>> u(7)=4
u =
   (1,7)        4

>> x=u+v
x =
   (1,2)        3
   (1,7)        4
```

```
>> dot(x,u)
ans =
   (1,1)       16
>> % The dot product of two sparse vectors is a sparse vector of length 1.

>> norm(x)
ans =
     5


>> w=[1:10]
w =
     1     2     3     4     5     6     7     8     9    10

>> w+v
ans =
     1     5     3     4     5     6     7     8     9    10
% Note that sparse and full vectors can be combined; the result is a full vector
```

2.6 Plotting vectors in MATLAB

One of the most useful and most complex aspects of MATLAB is its support for two- and three-dimensional graphics. In this book, we will discuss only the two-dimensional plotting system, and only the most basic aspects of that.

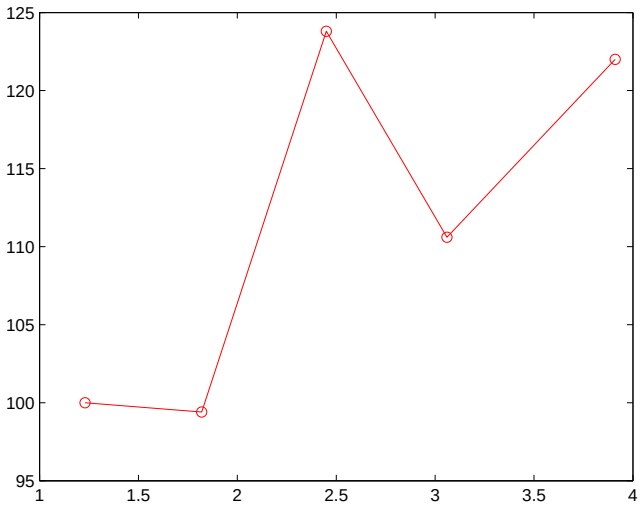
The basic plotting function is "plot". In its basic form, "`plot(x,y,c)`" takes as arguments two k-dimensional vectors, `x` and `y` and a control string `c`. It produces a plot of the points $\langle \mathtt{x}[1], \mathtt{y}[1] \rangle \ldots \langle \mathtt{x}[k], \mathtt{y}[1] \rangle$ in the display format indicated by control string `c`.

```
>> x=[1.23, 1.82, 2.45, 3.06, 3.91]
x =
    1.2300    1.8200    2.4500    3.0600    3.9100

>> y=[100, 99.4, 123.8, 110.6, 122]
y =
  100.0000   99.4000  123.8000  110.6000  122.0000

>> plot(x,y,'ro-')
```

The plot is output in a a MATLAB window called "Figure 1" shown here in figure 2.4. The figure can then be saved as a file in a variety of formats by using the "Save" or "SaveAs" option in the GUI associated with the plot window.

The plotting routine chooses "nice" ranges and tick frequencies for the x and y axes. The 'r' flag in the control string specifies color red; the 'o' flag specifies that the points are marked with circles, the '-' flag specifies that the points are connected with a solid line. Table 2.1 show other values for these specifiers.

The `saveas` function causes the current figure (denoted `gcf` to be saved in a format that can be reloaded into MATLAB. The `print` operation causes the current figure to be exported into .eps



In the online version of this book, this and other figures appear in color.
In the print version, they are reproduced in black-and-white.

Figure 2.4: Simple plot

Color		Point type		Line type	
`b`	blue	`*`	Asterisk	`-`	solid
`c`	cyan	`o`	Circle	`--`	dashed
`g`	green	`x`	Cross	`:`	dotted
`k`	black	`d`	Diamond	`-.`	dash-dot
`m`	magenta	`.`	Point		
`r`	red	`+`	Plus sign		
`w`	white	`s`	Square		
`y`	yellow	`<`	Left triangle		
		`>`	Right triangle		
		`^`	Up triangle		
		`v`	Down triangle		
		`p`	5 point star		
		`h`	6 point star		

Table 2.1: Specifiers for plotting

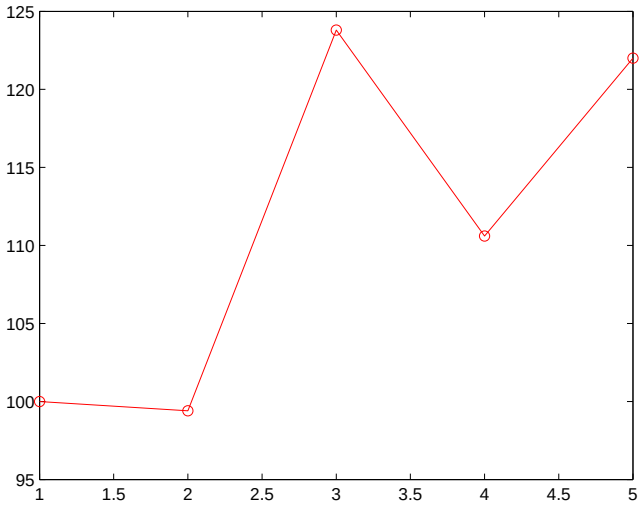


Figure 2.5: Using the default x-coordinates

format, suitable for use in LATEX. MATLAB supports exporting into a variety of formats, including .gif, .jpg, and so on.

The control parameters can be typed in any order within the control string. If any of the control parameters is omitted, then a default value is used. The default color is blue, the default data point indicator is none, the default line type is no line if a data point indicator is included and a solid line if it is not. For example:

> `plot(x,y)` — Points connected by blue line, no marker at points.
> `plot(x,y,'*g')` — Green points marked with asterisk; no line.
> `plot(x,y,'k:')` – Points connected by dotted black line, no marker at points.
> `plot(x,y,'--v')` — Blue points marked by downward triangle connected by blue dashed line.

If only one vector is specified, this is taken to be the vector of y coordinates, and it is plotted against the vector 1:k. For example, `plot(y,'ro-')` gives the plot in figure 2.5.

The next example illustrates the following three features:

- The plotted points need not be listed in increasing order of x coordinate. The lines connecting the points connect them in the order specified.
- The axes can be adjusted using the `axis` function.
- Multiple sequences of data points can be plotted on a single graph by calling plot with additional arguments: The call `plot(x1, y1, c1, x2, y2, c2, ...xn, yn, cn)` plots points `x1,y1` with control `c1`, `x2,y2` with control `c2`, and so on.

```
>> x=[1,5,5,1,1]
x =
     1     5     5     1     1
```

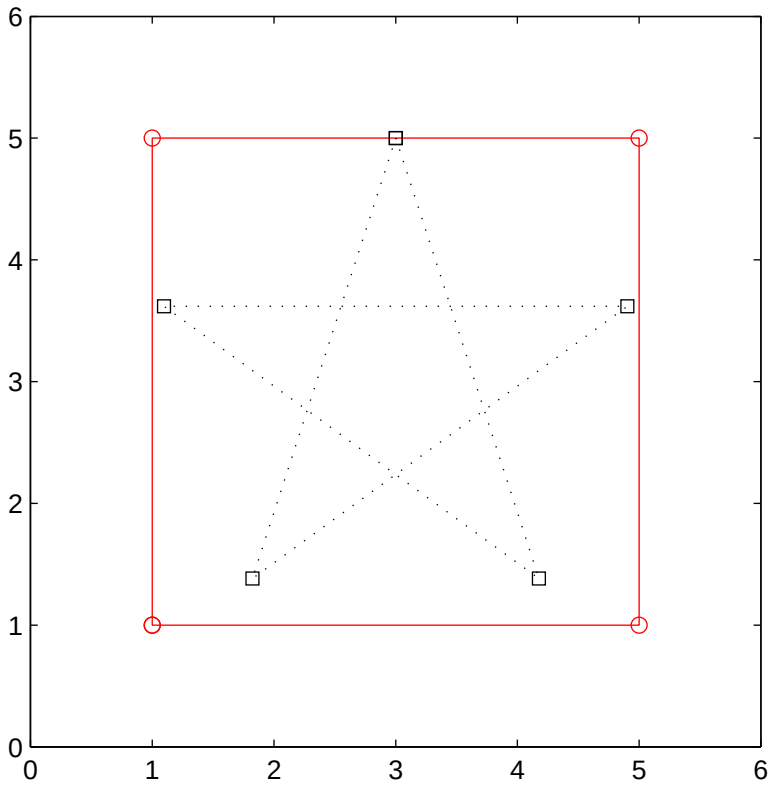


Figure 2.6: Plotting multiple data sets

```
>> y=[1,1,5,5,1]
y =
     1     1     5     5     1

>>  a=[3,3+2*sin(4*pi/5),3+2*sin(8*pi/5),3+2*sin(12*pi/5), 3+2*sin(16*pi/5),3]
a =
    3.0000    4.1756    1.0979    4.9021    1.8244    3.0000

>> b=[5,3+2*cos(4*pi/5),3+2*cos(8*pi/5),3+2*cos(12*pi/5), 3+2*cos(16*pi/5),5]
b =
    5.0000    1.3820    3.6180    3.6180    1.3820    5.0000
>> plot(x,y,'ro-',a,b,'ks:')
>> axis equal
>> axis([0,6,0,6])
```

The final plot is shown in figure 2.6. The "axis equal" command is useful with geometric plots to ensure equal spacing in the x- and y- dimensions.

The MATLAB graphics package has many, many more features including a GUI interface; look them

up as you want them.

2.7 Vectors in other programming languages

Almost every programming language supports one-dimensional and multi-dimensional arrays as primitive data structures.[7] One does, of course, have to be careful of the difference between 0-based indexing, used in language such as C and Java, and 1-based indexing, used in this book and in MATLAB.

Programming language support for sparse vectors is much less common. In most languages, a sparse vector $\vec{v}$ must be implemented as a set of pairs $\{\langle a_1, c_1\rangle \ldots \langle a_k, c_k\rangle\}$ where $c_1 \ldots c_k$ are the non-zero components of $\vec{v}$ and $a_1 \ldots a_k$ are the associated indices. For example, the vector $\vec{v} = [0, 0, 12, 0, -8, 12, 0, 0, 0, 0, 0]$ could be represented as the set $\{\langle 3, 12\rangle, \langle 5, -8\rangle, \langle 6, 12\rangle\}$.

Sets themselves, of course, can be implemented in a number of ways in conventional programming languages; and the choice of implementation here involves some tradeoffs. Consider, for example, the simple operation of indexing into a sparse vector; that is, finding $\vec{v}[i]$ given the set of pairs. If the set is implemented as a list, then the solution is to go through the pairs, until finding a pair $\langle a_j, c_j\rangle$ where $a_j = i$, and return c_j. However, this requires time proportional to the number of non-zero elements which can be large (the vector may still be sparse, if the dimensionality is enormous). Alternatively the set may be implemented as a hash table, which would support constant expected time indexing, but would complicate other operations.

Exercises

Exercise 2.1

Compute each of the following expressions by hand. Do not use MATLAB.

A. $3 \cdot \langle 1, -3, 2\rangle$.

B. $-2 \cdot \langle 4, 2, 0, 1\rangle$

C. $\langle 1, -3, 2\rangle + \langle 4, 2, 6\rangle$

D. $\langle 0, 1, 5, 2\rangle + \langle 1, -1, 1, -1\rangle$.

E. $\langle 1, -3\rangle \bullet \langle 4, 2\rangle$.

F. $\langle 1, -3, 2\rangle \bullet \langle 4, 2, 6\rangle$.

Exercise 2.2

Compute $|\langle 1, 1, 2\rangle|$ by hand. (You may leave this in the form "$\sqrt{x}$".)

[7] There have been programming languages, such as LISP and ML, whose early versions did not include arrays, but these have mostly acquired arrays as they became increasingly used for production software. Prolog has been resistant to arrays; there are dialects that include arrays, but most do not.

Exercise 2.3

By hand, find the cosine of the angle between $\langle 1, -3, 0\rangle$ and $\langle 2, 1, 3\rangle$. (You may leave this in the form "$x/(\sqrt{y}\sqrt{z})$".) Using MATLAB, find the actual angle.

Exercise 2.4

Let $\vec{u} = \langle 1, 4, -2\rangle$, $\vec{v} = \langle 2, 3, 5\rangle$, $\vec{w} = \langle -1, 4, 1\rangle$.

A. Verify by carrying out the calculation by hand that $\vec{u} \bullet (\vec{v} + \vec{w}) = (\vec{u} \bullet \vec{v}) + (\vec{u} \bullet \vec{w})$.

B. Compute $(\vec{u} \bullet \vec{v}) \cdot \vec{w}$ and $(\vec{w} \bullet \vec{v}) \cdot \vec{u}$. Are they equal?

Exercise 2.5

By hand, find the correlation between:

A. $\langle 1, 5, 3\rangle$ and $\langle 2, 10, 6\rangle$.

B. $\langle 1, 5, 3\rangle$ and $\langle 0, 1, 1\rangle$.

C. $\langle 1, 5, 3\rangle$ and $\langle 5, 1, 3\rangle$.

Problems

Problem 2.1

Find three two-dimensional vectors $\vec{u} \neq \vec{0}, \vec{v}, \vec{w}$ such that $\vec{u} \bullet \vec{v} = \vec{u} \bullet \vec{w}$ but $\vec{v} \neq \vec{w}$.

Problem 2.2

Prove the algebraic properties of the basic operations on vectors stated in section 2.3.1.

Problem 2.3

Prove the algebraic properties of the basic operations on vectors stated in section 2.4.1.

Programming Assignments

Assignment 2.1: Document Vectors

Write a MATLAB function `DocSimilarity(D,E)` which computes the "similarity" of text documents D and E using the vector model of documents. Specifically, the arguments D and E are each cell arrays of strings, each string being a word of the document, normalized to lower case. (Cell arrays are heterogeneous arrays. See section 3.10.2.) The function returns a number between 0 and 1, 0

meaning that the two documents have no two significant words in common, 1 meaning that they have the identical significant words with the same frequency.

A word is considered "significant" if it has at least three letters and is not in the list of stop words provided at SampleCode/GetStopwords.m on the course web site.

A stop word is a very common word that should be ignored.

Your function should execute the following steps.

- Let LargeOdd be any reasonably large odd number that is not very close to a power of 256. 10,000,001 will do fine.
- Load in the cell array of stop words from GetStopwords.m
- Create three sparse vectors $\vec{S}, \vec{D}, \vec{E}$ of size LargeOdd, as follows: For every word W, let i=hash(W,LargeOdd). You can find a hash function at SampleCode/hash.m. Then
  - $\vec{S}[i] = 1$ if W is on the list of stop words.
  - $\vec{D}[i]$ = the number of occurences of W in D, if W is significant.
  - $\vec{E}[i]$ = the number of occurences of W in E, if W is significant.

  (Create $\vec{S}$ first, then use it for a quick test for whether words in the documents are significant.) $\vec{D}$ and $\vec{E}$ are the document vectors (we omit the inverse document frequency).
- Return the quantity $\vec{D} \bullet \vec{E}/|\vec{D}| \cdot |\vec{E}|$

For instance,

```
>> D = { 'how', 'much', 'wood', 'could', 'a', 'woodchuck', 'chuck',  ...
'if', 'a', 'woodchuck', 'could', 'chuck', 'wood' };
>> E = { 'all', 'the', 'wood', 'that', 'a', 'woodchuck', 'could',  ...
'if', 'a', 'woodchuck', 'could', 'chuck', 'wood' };
>> DocSimilarity(D,E)
ans =
  0.9245
```

Note that the only significant words in these two texts are "chuck", "much", "wood", and "woodchuck".

You don't have to worry about hash collisions, because they are very infrequent, and the technique is completely imprecise in any case.

Assignment 2.2: Plotting the harmonic series

The harmonic function $H(n)$ is defined as $H(n) = \sum_{i=1}^{n} 1/n$. For instance $H(4) = 1/1+1/2+1/3+1/4 = 25/12 = 2.1666$. For large n, $H(n)$ is approximately equal to $\ln(n) + \gamma$, where $\ln(n)$ is the natural logarithm and $\gamma = 0.5772$, known as Euler's constant.

Write a MATLAB function `PlotHarmonic(N)` that shows both $H(k)$ and $\ln(k) + \gamma$ for $k = 1 \ldots N$.

Assignment 2.3: Correlation to a noisy signal

Write a MATLAB function `CorrelationNoisy(V,E)` as follows. The input parameters are `V`, a vector, and `E`, a positive real. The function constructs a new vector `U` by adding a random number between $-$`E` and `E` to each component of `V` (a different random choice for each component; use the function `rand`.) It then returns the correlation between `V` and `U`.

Experiment with `V` = `1 : 100` and various value of `E`. Run each value of `E` several times to get a range of correlations. What kind of values do you get for the correlation when `E` = 10? When `E` = 100? How large do you have to make `E` before you start to see examples with negative correlations?

Assignment 2.4: Stars

An n-pointed regular star can be constructed as follows:

- Choose $k > 1$ relatively prime to n.
- Place the ith vertex of the star at $x_i = \cos(2\pi ki/n), y_i = \cos(2\pi ki/n)$ for $i = 0, n$. Note that $\langle x_n, y_n \rangle = \langle x_0, y_0 \rangle$, so the star closes.

Write a MATLAB function `Star(N,K)` which draws this N pointed star. Be sure to call `axis equal` so that the x- and y- axes are drawn with equal scale; otherwise, the star will be oddly squooshed.

Assignment 2.5: Euler's sieve

Euler's sieve is a souped-up version of the sieve of Eratosthenes, which finds the prime numbers. It works as follows

```
L = the list of numbers from 2 to N;
P = 2; /* The first prime */
while (P^{2} < N) {
   L1 = the list of all X in L  such that P $\leq$ X $\leq$ N/P.
   L2 = P*L1;
   delete everything in L2 from L;
   P = the next value after P in L;
   }
return L;
```

For instance, for N=27, successive iterations proceed as follows:

```
Initialization
  L = [2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27]
  P = 2

First iteration
  L1 = [2 3 4 5 6 7 8 9 10 11 12 13]
  L2 = [4 6 8 10 12 14 16 18 20 22 24 26]
  L = [2 3 5 7 9 11 13 15 17 19 21 23 25 27]
  P = 3
```

```
Second iteration
  L1 = [3 5 7 9]
  L2 = [9 15 21 27]
  L = [2 3 5 7 11 13 17 19 23 25]
  P = 5

Third iteration
  L1 = [5]
  L2 = [25]
  L = [2 3 5 7 11 13 17 19 23]
```

A. Write a MATLAB function `EulerSieve1(N)` which constructs the Euler sieve, implementing L, L1, L2 as arrays of integers, as above.

B. Write a MATLAB function `EulerSieve2(N)` which constructs the Euler sieve, implementing L, L1, and L2 as Boolean arrays, where L[I] = 1 if I is currently in the set L. Thus, the final value returned in the above example would be the array

```
[0 1 1 0 1 0 1 0 0 0 1 0 1 0 0 0 1 0 1 0 0 0 1 0 0 0 0]
```

Chapter 3

Matrices

3.1 Definition of matrices

A $m \times n$ *matrix* is a rectangular array of numbers with m rows each of length n; equivalently, n columns, each of length m.

Example:

$$A = \begin{bmatrix} 4 & 2 & -1 \\ 0 & 6 & 5 \end{bmatrix} \text{ is a } 2 \times 3 \text{ array.} \qquad B = \begin{bmatrix} 0 & -1.5 \\ 2.1 & 6 \\ -1.0 & -3.5 \\ 1.0 & 2.2 \end{bmatrix} \text{ is a } 4 \times 2 \text{ array}$$

We will use capital italic letters, such as M, for matrices. The element in the ith row, jth column in matrix M is denoted $M[i, j]$. For instance, in the matrices above, $A[2, 1] = 0$. $A[1, 3] = -1$. $B[2, 1] = 2.1$. $B[3, 2] = -3.5$.

There is no very standard notation for specifying a particular row or column of a matrix. Following MATLAB, we will use the notation $M[i, :]$ for the ith row of M (a row vector) and $M[:, j]$ for the jth column. (MATLAB uses parentheses rather than square brackets, however.)

3.2 Applications of matrices

The simplest types of $m \times n$ matrices are those whose m rows are just n-dimensional vectors of the types discussed in chapter 2, or whose n columns are m-dimensional vectors. In particular, if one has an application of category (3) as discussed in section 2.2.1, in which there is a numeric function of two entities or features, then this can be represented as a matrix in the obvious way: Given two set of entities/features $\{O_1 \ldots O_m\}$ and $\{P_1 \ldots P_n\}$ and a numeric function $f(O, P)$, construct the $m \times n$ matrix M such that $M[i, j] = f(O_i, P_j)$

For example, in the grocery shopping application (4), suppose we have a set of people { Amy, Bob, Carol } and a set of grocery items { gallon of milk, pound of butter, apple, carrot } then we can define a 3×4 array, S where $S[i, j]$ is the number of items of type j on i's shopping list.

$$S = \begin{bmatrix} 0 & 2 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 6 \end{bmatrix}$$

Thus Amy is buying 2 pounds of butter and an apple; Bob is buying a gallon of milk and a pound of butter; and Carol is buying a gallon of milk and six carrots.

Note that each row of this matrix is the row vector corresponding to one person p; it shows p's shopping list indexed by item. Each column of this matrix is the column vector corresponding to one item i; it shows the quantity of that product being bought, indexed by person.

If the collection of grocery items indexed is large, then this will be a *sparse matrix*, that is, a matrix most of whose entries are 0.

In application 2 of time series, if you have r different financial measures that you are tracking over m days, then this data could be recorded in a $m \times n$ matrix P, where $P[i, j]$ is the value of measure i on day j.

Particular interesting are cases where the two sets of entities $\{O_1 \dots O_n\}$ and $\{P_1 \dots P_n\}$ are the same. In this case, the resulting matrix is a $n \times n$ matrix, called a *square* matrix.

Application 11: Distance graph. For instance, one could have a collection of n cities, and define a $n \times n$ matrix D where $D[i, j]$ is the distance from i to j. In general, a directed graph (in the data structures sense) over n vertices can be represented as an $n \times n$ adjacency matrix where $A[i, j] = 1$ if there is an arc from i to j and 0 if there is not. A graph with numeric labels on its arcs can be represented as a $n \times n$ matrix where $A[i, j]$ is the label on the arc from i to j.

Application 12: Functions over a rectangular region. A different category of matrix represents a numeric function over a planar region. This can be done by picking out a rectangular $m \times n$ grid of points, and constructing a $m \times n$ matrix M where $M[i, j]$ is the value of the function at point i, j. In particular an *image*, either output for graphics or input for computer vision, is represented in terms of such a grid of pixels. A gray-scale image is represented by a single array I, where $I[i, j]$ is the intensity of light, often encoded as an 8-bit integer from 0 (black) to 255 (white), at the point with coordinates $\langle i, j \rangle$. A color image is represented by three matrices, representing the intensity of light at three different component frequencies.

From the standpoint of linear algebra, these kinds of arrays are actually atypical examples of matrices, since most of the important operations on images do not correspond very closely to the standard operations of linear algebra. In section 6.4.8 we will briefly discuss how geometric transformations are applied to pixel arrays.

3.3 Simple operations on matrices

The product of a matrix by a scalar and the sum of two matrices is computed component by component, as with vectors. That is,

$$(a \cdot M)[i, j] = a \cdot M[i, j].$$

$$\text{E.g. } 3 \cdot \begin{bmatrix} 3 & 1 & 2 \\ 0 & -1 & 4 \end{bmatrix} = \begin{bmatrix} 3 \cdot 3 & 3 \cdot 1 & 3 \cdot 2 \\ 3 \cdot 0 & 3 \cdot -1 & 3 \cdot 4 \end{bmatrix} = \begin{bmatrix} 9 & 3 & 6 \\ 0 & -3 & 12 \end{bmatrix}$$

$$(M + N)[i, j] = M[i, j] + N[i, j].$$

$$\text{E.g. } \begin{bmatrix} 3 & 1 & 2 \\ 0 & -1 & 4 \end{bmatrix} + \begin{bmatrix} 7 & -2 & 3 \\ 5 & 6 & 2 \end{bmatrix} = \begin{bmatrix} 3+7 & 1-2 & 2+3 \\ 0+5 & -1+6 & 4+2 \end{bmatrix} = \begin{bmatrix} 10 & -1 & 5 \\ 5 & 5 & 6 \end{bmatrix}$$

The *transpose* of matrix M, denoted M^T, turns the rows of M into columns and vice versa. That is, if M is a $m \times n$ matrix, then M^T is an $n \times m$ matrix, and $M^T[i,j] = M[j,i]$. For instance,

$$\text{If } A = \begin{bmatrix} 4 & 2 & -1 \\ 0 & 6 & 5 \end{bmatrix} \text{ then } A^T = \begin{bmatrix} 4 & 0 \\ 2 & 6 \\ -1 & 5 \end{bmatrix}$$

The following properties are immediate from the definitions: (In all of the following M, N, and P are $m \times n$ matrices and a and b are scalars.)

$M + N = N + M$.
$M + (N + P) = (M + N) + P$
$a(M + N) = aM + aN$
$(a + b)M = aM + bM$.
$(ab)M = a(bM)$.
$(M^T)^T = M$.
$M^T + N^T = (M + N)^T$.
$aM^T = (aM)^T$.

3.4 Multiplying a matrix times a vector

Let M is a $m \times n$ matrix and let $\vec{v}$ be a n-dimensional vector. The product $M \cdot \vec{v}$ is a m-dimensional vector consisting of the dot products of each row of M with $\vec{v}$. That is, $(M \cdot \vec{v})[i] = M[i,:] \bullet \vec{v} = \sum_{j=1}^{n} M[i,j] \cdot \vec{v}[j]$. For instance,

$$\text{If } M = \begin{bmatrix} 3 & 1 & 2 \\ 0 & -1 & 4 \end{bmatrix} \text{ and } \vec{v} = \langle 2, -1, 4 \rangle \text{ then}$$

$$M\vec{v} = \langle M[1,:] \bullet \vec{v},\ M[2,:] \bullet \vec{v} \rangle = \langle (3 \cdot 2) + (1 \cdot -1) + (2 \cdot 4),\ (0 \cdot 2) + (-1 \cdot -1) + (4 \cdot 4) \rangle = \langle 13, 17 \rangle$$

Generally, for reasons we will soon come to, when one writes out the product of a matrix times a vector, both vectors (the multiplicand and the product) are written as column vectors, thus:

$$\begin{bmatrix} 3 & 1 & 2 \\ 0 & -1 & 4 \end{bmatrix} \cdot \begin{bmatrix} 2 \\ -1 \\ 4 \end{bmatrix} = \begin{bmatrix} 13 \\ 17 \end{bmatrix}$$

Written in this way, one uses the "two-hands" method for computing the product; the left hand moves from left to right along each row of the matrix while the right hand moves from top to bottom along the vector.

The order is critical here; $\vec{v} \cdot M$ means something quite different from $M \cdot \vec{v}$, as we will soon discuss.

The following algebraic rules on multiplication of matrices times vectors follow immediately from the rules about dot products discussed in section 2.4.1. In all the following M and N are $m \times n$ matrices; $\vec{u}$ and $\vec{v}$ are n-dimensional vectors; and a is a scalar.

$(M + N)\vec{v} = M\vec{v} + N\vec{v}$
$M(\vec{u} + \vec{v}) = M\vec{u} + M\vec{v}$
$(aM)\vec{v} = a(M\vec{v}) = M(a\vec{v})$

The product $M \cdot \vec{v}$ can also be described as the weighted sum of the columns of M, where the weights are the components of $\vec{v}$.

$$M \cdot \vec{v} = \vec{v}[1] \cdot M[:, 1] + \ldots + \vec{v}[n] \cdot M[:, n]$$

For instance

$$\begin{bmatrix} 3 & 1 & 2 \\ 0 & -1 & 4 \end{bmatrix} \cdot \begin{bmatrix} 2 \\ -1 \\ 4 \end{bmatrix} = 2 \cdot \begin{bmatrix} 3 \\ 0 \end{bmatrix} + -1 \cdot \begin{bmatrix} 1 \\ -1 \end{bmatrix} + 4 \cdot \begin{bmatrix} 2 \\ 4 \end{bmatrix} = \begin{bmatrix} 13 \\ 17 \end{bmatrix}$$

As we will see, the equivalence of these two dual ways of describing $M \cdot v$ – the dot product of the rows of M with $\vec{v}$ or the sum of the columns of M weighted by the components of $\vec{v}$ — has deep consequences.

3.4.1 Applications of multiplying a matrix times a vector

The **geometric applications** are very important and interesting, but too complex for a short discussion here. These are discussed in chapter 6.

The simplest applications of $M \cdot \vec{v}$ are those where you are interested separately in the dot product of each of the rows with the vector. For instance, in application 4 of grocery shopping, let B be a matrix of shopping baskets; $B[i, j]$ is the number of item j that person i is buying. Let $\vec{p}$ be a vector of prices; $\vec{p}[j]$ is the price of item j. Then $B \cdot \vec{p}$ is a vector of total cost for each person; that is, $(B \cdot \vec{p})[i]$ is the cost of the shopping basket for person i.

Similarly, let P be a matrix of prices of items at stores; $P[i, j]$ is the price of item j at store i. Let $\vec{b}$ be the vector of a shopping basket; $\vec{b}[j]$ is the number of item j to be bought. Then $P \cdot \vec{b}$ is the vector of the cost of the basket by store; that is $(P \cdot \vec{b})[i]$ is the cost of the shopping basket at store i.

More interesting, perhaps, are the applications in which M represents a transformation of the vector as a whole.

Application 13: Transition matrix

Let $\vec{v}$ represent the populations of a collection of cities at a given time. Let M be an annual *transition* matrix for populations. That is, for any two cities i and j, if $i \neq j$, $M[i, j]$ is the fraction of the inhabitants of j who move to i. $M[i, i]$ is the fraction of the inhabitants of i who remain at i. (We will ignore births and deaths.) What is the population of city i after a year? First, there are the people who stayed in i; there are $M[i, i] \cdot \vec{v}[i]$ of these. Then there are the people who immigrated to i; from each city j, the number of people who have immigrated to i is $M[i, j]\vec{v}[j]$. Therefore, the total number of people in i is $\sum_j M[i, j] \cdot \vec{v}_[j] = M[i, :] \bullet \vec{v}$. Therefore $M\vec{v}$ is the vector of populations after a year.

For instance, suppose there are three cities A, B, and C, with the following transitions:

- Of the population of A, 70% remain in A; 20% move to B, and 10% move to C.
- Of the population of B, 25% move to A; 65% remain in B, and 10% move to C.
- Of the population of C, 5% move to A; 5% move to B, and 90% remain in C.

Thus, the transition matrix is

$$\begin{bmatrix} 0.7 & 0.25 & 0.05 \\ 0.2 & 0.65 & 0.05 \\ 0.1 & 0.1 & 0.9 \end{bmatrix}$$

If initially there are 400,000 people in A, 200,000 in B, and 100,000 in C then after a year the population vector will be given by

$$\begin{bmatrix} 0.7 & 0.25 & 0.05 \\ 0.2 & 0.65 & 0.05 \\ 0.1 & 0.1 & 0.9 \end{bmatrix} \cdot \begin{bmatrix} 400,000 \\ 200,000 \\ 100,000 \end{bmatrix} = \begin{bmatrix} 335,000 \\ 215,000 \\ 150,000 \end{bmatrix}$$

Note that each column of the matrix adds up to 1; this corresponds to the fact that total number of people remains constant. A matrix whose columns add to 1 is known as a *stochastic* matrix; we will study these in greater depth in chapter 10.

Application 14: Smoothing a signal

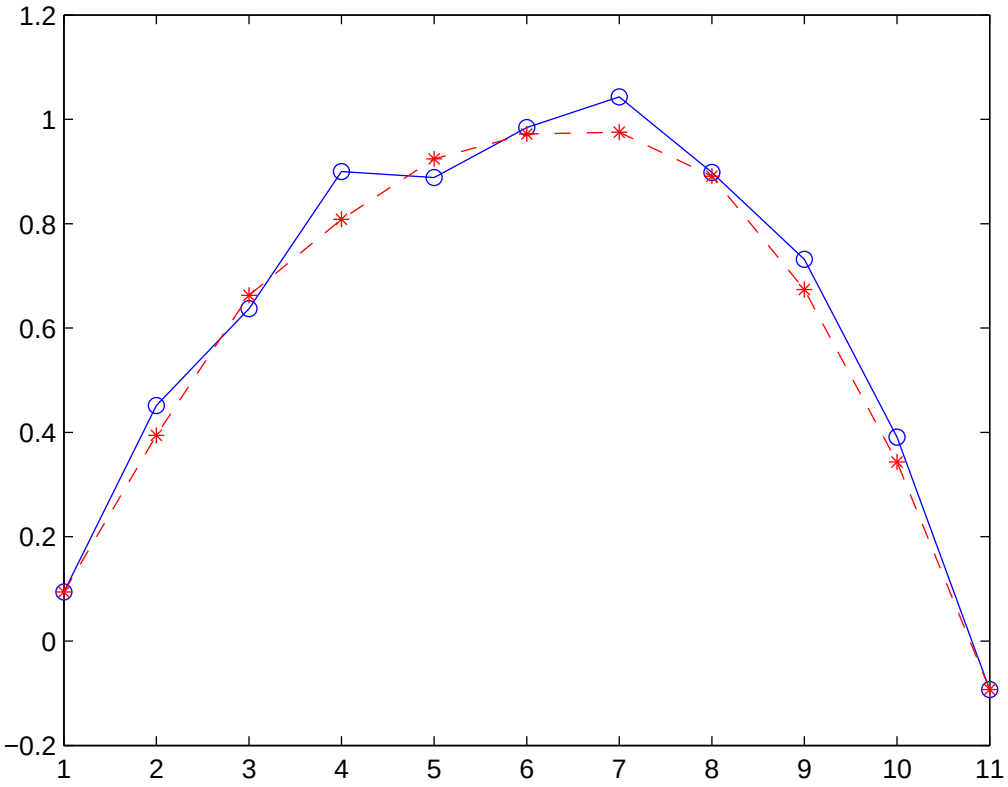
Let $\vec{v}$ be a time sequence of a numeric quantity, as in application 2. Suppose that we wish to eliminate noise from a signal. One standard way to do this is to estimate the true value of the signal at each point of time by the weighted average of the signal at nearby points; this is known as *smoothing* the signal. The width of the range depends both on the frequencies of the noise and the signal and on the signal to noise ratio; ideally you want to average over a range larger than the wavelength of the noise, smaller than the wavelength of the signal, and over a set of points large enough that the noise will average out to zero.

Let $\vec{d}[t]$ be the data at time t and let $\vec{s}[t]$ be the estimate of the signal. If the signal frequency is very high, and the noise is fairly small, then one might estimate the signal at time t, $\vec{q}[t] = 1/3 \cdot (\vec{d}[t-1] + \vec{d}[t] + \vec{d}[t+1])$. Of course, at the beginning of the time range where $\vec{d}[t-1]$ is not recorded, and at the end where $\vec{d}[t+1]$ is not recorded, one has to do something different; what we will do is just set $\vec{q}[1] = \vec{d}[1]$ and $\vec{q}[k] = \vec{d}[k]$.

Each of these sums is a weighted average of the data; the entire transformation of signal to noise is thus the multiplication of the data vector by a smoothing matrix. For instance, let us consider the following artificial data. The true signal $\vec{s}$ is just the quadratic function $\vec{s}[i] = 1 - ((i-6)/5)^2$ for $i = 1 \ldots 11$; thus $\vec{s} = \langle 0, 0.36, 0.64, 0.84, 0.96, 1, 0.96, 0.84, 0.64, 0.36, 0 \rangle$. The noise $\vec{n}$ is generated by the MATLAB expression `(0.2 * rand(1,11)) - 0.1`. The data $\vec{d} = \vec{s} + \vec{n} = \langle 0.0941, 0.4514, 0.6371, 0.9001, 0.8884, 0.9844, 1.0431, 0.8984, 0.7319, 0.3911, -0.0929 \rangle$

We smooth the data by carrying out the following multiplication (figure 3.1):

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1/3 & 1/3 & 1/3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/3 & 1/3 & 1/3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/3 & 1/3 & 1/3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/3 & 1/3 & 1/3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/3 & 1/3 & 1/3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/3 & 1/3 & 1/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1/3 & 1/3 & 1/3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/3 & 1/3 & 1/3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/3 & 1/3 & 1/3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 0.0941 \\ 0.4514 \\ 0.6371 \\ 0.9001 \\ 0.8884 \\ 0.9844 \\ 1.0431 \\ 0.8984 \\ 0.7319 \\ 0.3911 \\ -0.0929 \end{bmatrix} = \begin{bmatrix} 0.0941 \\ 0.3942 \\ 0.6629 \\ 0.8085 \\ 0.9243 \\ 0.9720 \\ 0.9753 \\ 0.8912 \\ 0.6738 \\ 0.3434 \\ -0.0929 \end{bmatrix}$$



The noisy points are the circles on the solid blue line.
The smoothed points are the asterisks on the dashed red line.

Figure 3.1: Smoothing

The correlation of the data with the ideal signal is 0.9841. The correlation of the smoothed data with the ideal signal is 0.9904.

Application 15: Time-shifting a signal

Another operation on time sequences that can be modelled as matrix multiplication is time shifting. Suppose you have a signal $\vec{s}$ of length n and wish to construct the same signal shifted q units later; that is, $\vec{z}[i] = \vec{z}[i-q]$. This can be viewed as multiplication by an $n \times n$ matrix M such that $M[i+q, i] = 1$ for $i = q+1 \ldots n$ and $M[i, j] = 0$ for all $j \neq i+q$. For example, with $n = 6$, $q = 2$,

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} 2 \\ 8 \\ 5 \\ 7 \\ 1 \\ 4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 2 \\ 8 \\ 5 \\ 7 \end{bmatrix}$$

This may seem like an awfully elaborate and verbose way of formulating a very simple operation, and if all you want to do is a time shift, it certainly would be. But the point is that you can then combine it with other matrix operations and apply the results of matrix theory to these combinations.

Application 16: Jacobians (Optional)

(Note: This requires multivariable calculus.)

Suppose $\mathbf{F}(\mathbf{p})$ is a differentiable function from the plane to itself. We will write $\mathbf{F}_x$ and $\mathbf{F}_y$ for the x and y components of $\mathbf{F}$. For example, if $\mathbf{F}(\langle x, y\rangle) = \langle x + y, x^2 - y^2\rangle$, then $\mathbf{F}_x(\langle x, y\rangle) = x + y$ and $\mathbf{F}_y(\langle x, y\rangle) = x^2 - y^2$.

We're going to take a particular point $\mathbf{a}$, draw tiny vectors with their tails at $\mathbf{a}$, and consider the mapping $\mathbf{F}$ does to those vectors. So let $\epsilon > 0$ be a very small distance, let $\vec{u}$ be a vector, and let $\mathbf{b} = \mathbf{a} + \epsilon\vec{u}$. Let u_x and u_y be the coordinates of $\vec{u}$ in the x and y directions. Thus $\vec{u} = u_x\hat{x} + u_y\hat{y}$ where $\hat{x}$ and $\hat{y}$ are the unit x and y vectors. We have $\mathbf{b} = \mathbf{a} + \epsilon u_x\hat{x} + \epsilon u_y\hat{y}$.

Now what is $\mathbf{F}(\mathbf{b})$? By the definition of the partial derivative,

$$\mathbf{F}_x(\mathbf{a} + \epsilon u_x\hat{x}) - \mathbf{F}_x(\mathbf{a}) \approx \epsilon u_x \cdot \frac{\partial \mathbf{F}_x}{\partial x}$$

and

$$\mathbf{F}_x(\mathbf{a} + \epsilon u_x\hat{x} + \epsilon u_y\hat{y}) - \mathbf{F}_x(\mathbf{a} + \epsilon u_x\hat{x}) \approx \epsilon u_y \cdot \frac{\partial \mathbf{F}_x}{\partial y}$$

So adding these together

$$\mathbf{F}_x(\mathbf{b}) - \mathbf{F}_x(\mathbf{a}) = \mathbf{F}_x(\mathbf{a} + \epsilon u_x\hat{x} + \epsilon u_y\hat{y}) - \mathbf{F}_x(\mathbf{a}) \approx \epsilon(u_x \cdot \frac{\partial \mathbf{F}_x}{\partial x} + u_y \cdot \frac{\partial \mathbf{F}_x}{\partial y})$$

Likewise

$$\mathbf{F}_y(\mathbf{b}) - \mathbf{F}_y(\mathbf{a}) = \mathbf{F}_y(\mathbf{a} + \epsilon u_x\hat{x} + \epsilon u_y\hat{y}) - \mathbf{F}_y(\mathbf{a}) \approx \epsilon(u_x \cdot \frac{\partial \mathbf{F}_y}{\partial x} + u_y \cdot \frac{\partial \mathbf{F}_y}{\partial y})$$

Let $\vec{w} = (\mathbf{F}(\mathbf{b}) - \mathbf{F}(\mathbf{a}))/\epsilon$ so $\mathbf{F}(\mathbf{b}) = \mathbf{F}(\mathbf{a}) + \epsilon\vec{w}$. Then we have

$$\vec{w} = (u_x \cdot \frac{\partial \mathbf{F}_x}{\partial x} + u_y \cdot \frac{\partial \mathbf{F}_x}{\partial y})\hat{x} + (u_x \cdot \frac{\partial \mathbf{F}_y}{\partial x} + u_y \cdot \frac{\partial \mathbf{F}_y}{\partial y})\hat{y} = \begin{bmatrix} \frac{\partial \mathbf{F}_x}{\partial x} & \frac{\partial \mathbf{F}_x}{\partial y} \\ \\ \frac{\partial \mathbf{F}_y}{\partial x} & \frac{\partial \mathbf{F}_y}{\partial y} \end{bmatrix} \cdot \vec{u}$$

The 2×2 matrix in the last expression above is known as the *Jacobian* of $\mathbf{F}$, notated $J(\mathbf{F})$

For example, let $\mathbf{F}$ be as above, let $\mathbf{a} = \langle 2, 3\rangle$, let $\vec{u} = \langle 5, 2\rangle$ and let $\epsilon = 0.001$. Thus $\mathbf{b} = \langle 2.005, 3.002\rangle$ and $\mathbf{F}(\mathbf{a}) = \langle 5, -5\rangle$.

$$J(\mathbf{F}) = \begin{bmatrix} \frac{\partial \mathbf{F}_x}{\partial x} & \frac{\partial \mathbf{F}_x}{\partial y} \\ \\ \frac{\partial \mathbf{F}_y}{\partial x} & \frac{\partial \mathbf{F}_y}{\partial y} \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ \\ x & -y \end{bmatrix}$$

So

$$\mathbf{F}(\mathbf{b}) \approx \mathbf{F}(\mathbf{a}) + J(\mathbf{F})|_{\mathbf{a}} \cdot \epsilon\vec{u} = \begin{bmatrix} 5 \\ -5 \end{bmatrix} + \begin{bmatrix} 1 & 1 \\ 2 & -3 \end{bmatrix} \begin{bmatrix} 0.005 \\ 0.002 \end{bmatrix} = \begin{bmatrix} 5.007 \\ -4.996 \end{bmatrix}$$

We can generalize this to space of arbitrary dimension. Let $\mathbf{F}(\mathbf{p})$ be a differentiable function from $\mathbb{R}^n$ to $\mathbb{R}^m$. Let $\mathbf{a}$ be a point in $\mathbb{R}^n$, let $\epsilon > 0$ be small, let $\vec{u}$ be a vector in $\mathbb{R}^n$, and let $\mathbf{b} = \mathbf{a} + \epsilon\vec{u}$. Let $\hat{x}_1 \dots \hat{x}_n$ be the coordinate vectors of $\mathbb{R}^n$, and let $\mathbf{F}_1 \dots \mathbf{F}_m$ be the components of $\mathbf{F}$. Then

$$\mathbf{F}(\mathbf{b}) \approx \mathbf{F}(\mathbf{a}) + \begin{bmatrix} \frac{\partial \mathbf{F}_1}{\partial x_1} & . & . & . & \frac{\partial \mathbf{F}_1}{\partial x_n} \\ . & . & & . & . \\ . & & . & & . \\ . & . & & . & . \\ \frac{\partial \mathbf{F}_m}{\partial x_1} & . & . & . & \frac{\partial \mathbf{F}_m}{\partial x_n} \end{bmatrix} \cdot \epsilon\vec{u}$$

Again this array is called the Jacobian.

3.5 Linear transformation

Like dot product, the fundamental significance of matrix multiplication is that it is a linear transformation.

Definition 3.1. *Let $f(\vec{v})$ be a function from $\mathbb{R}^n$, the set of n-dimensional vectors to $\mathbb{R}^m$, the set of m-dimensional vectors. We say that f is a* linear transformation *if it satisfies the following two properties:*

- *For any vector $\vec{v}$ and scalar a, $f(a \cdot \vec{v}) = a \cdot f(\vec{v})$.*
- *For any vectors $\vec{v}, \vec{u}$, $f(\vec{v} + \vec{u}) = f(\vec{v}) + f(\vec{u})$.*

Theorem 3.1. *Let f be a linear transformation from $\mathbb{R}^n$ to $\mathbb{R}^m$. Then there exists a unique $m \times n$ matrix F, such that, for all $\vec{v}$, $f(\vec{v}) = F \cdot \vec{v}$. We say that matrix F* corresponds *to transformation f, and vice versa.*

Note that definition 3.1 is word for word identical to definition 2.1 except that the range of the function f has been changed from the real numbers $\mathbb{R}$ to $\mathbb{R}^m$. Theorem 3.1 is the same as theorem 2.1 except that the range has been changed, and "dot product with $\vec{f}$" has been changed to "multiplication by matrix F".

The proof is also essentially identical. Now we must imagine that we have a personal shopper to whom we give a basket $\vec{b}$ over a space of m groceries, and who reports back a vector $f(\vec{b})$ of the price of this basket at m different stores. The unit vector $\vec{e}^{\,i}$ corresponds the basket containing the one unit of the ith item. Then $f(\vec{e}^{\,i})$ is the vector showing the price of the ith item at all the stores. Construct the matrix $m \times n$ matrix F so that $F[i, j] = f(\vec{e}^{\,j})[i]$. Now let $\vec{b} = \langle b_1 \dots b_m\rangle$ be any

m-dimensional matrix. We can write $\vec{b} = b_1\vec{e}^{\,1} + \ldots + b_m\vec{e}^{\,m}$ so, by linearity, the ith component of $f(\vec{b})$,

$$f(\vec{b})[i] = f(\sum_j b_j \cdot \vec{e}^{\,j})[i] = \sum_j b_j \cdot (f(\vec{e}^{\,j})[i]) = \sum_j b_j \cdot F[i,j] = F[i,:] \bullet \vec{b}$$

Therefore $f(\vec{b}) = F \cdot \vec{b}$.

The duality here between linear transformations and matrices is the key to linear algebra. Theorem 3.1 means that we can go back and forth between thinking about linear transformations over vector spaces and multiplying vectors by matrices, and transfer results from each view to the other.

The one critical place where the correspondence does not work very well is in matrix transposition. Forming the transpose of a matrix is a simple operation on matrices and, as we shall see, an important one; but it does not correspond to anything very simple in terms of the linear transformations involved.

It should be noted that there are many simple and important functions on vectors that are not linear transformations, such as the function "max($\vec{v}$)", which returns the largest component of vector $\vec{v}$; the function "sort($\vec{v}$)", which returns the components of $\vec{v}$ in increasing order; and the function "product($\vec{v}$)", which returns the product of the components of $\vec{v}$. We leave the proof that none of these is a linear transformation to the reader (problem 3.4).

3.6 Systems of linear equations

A system of m linear equations in n unknowns is a set of equations of the form

$$a_{1,1}x_1 + a_{1,2}x_2 + \ldots + a_{1,n}x_n = c_1.$$

$$a_{2,1}x_1 + a_{2,2}x_2 + \ldots + a_{2,n}x_n = c_2.$$

$$\ldots$$

$$a_{m,1}x_1 + a_{m,2}x_2 + \ldots + a_{m,n}x_n = c_m.$$

Here all the $a_{i,j}$ and the c_i are constants, and the x_i are variables. A *solution* to the system is a set of values for the x_i that satisfies all the equations. The values $a_{i,j}$ are called the *coefficients* of the system; the values c_j are called the *constant terms*.

For example the following is a system of 3 equations in 4 unknowns:

$$\begin{array}{rcrcrcrcr} 1\cdot w & + & 1\cdot x & + & 1\cdot y & + & 1\cdot z & = & 2. \\ 2\cdot w & + & 0\cdot x & - & 1\cdot y & + & 3\cdot z & = & -1. \\ -1\cdot w & + & 2\cdot x & + & 0\cdot y & + & 1\cdot z & = & 2. \end{array}$$

One solution to this system is $w = 1, x = 2, y = 0, z = -1$, as can be seen by substituting in and checking the equations. Another solution is $w = 2, x = 3, y = -1, z = -2$.

A system of linear equations can be written as a problem in matrix multiplication. Let

$$A = \begin{bmatrix} a_{1,1} & \ldots & a_{1,n} \\ . & & . \\ . & & . \\ . & & . \\ a_{m,1} & \ldots & a_{m,n} \end{bmatrix} \quad X = \begin{bmatrix} x_1 \\ . \\ . \\ . \\ x_n \end{bmatrix} \quad C = \begin{bmatrix} c_1 \\ . \\ . \\ . \\ c_m \end{bmatrix}$$

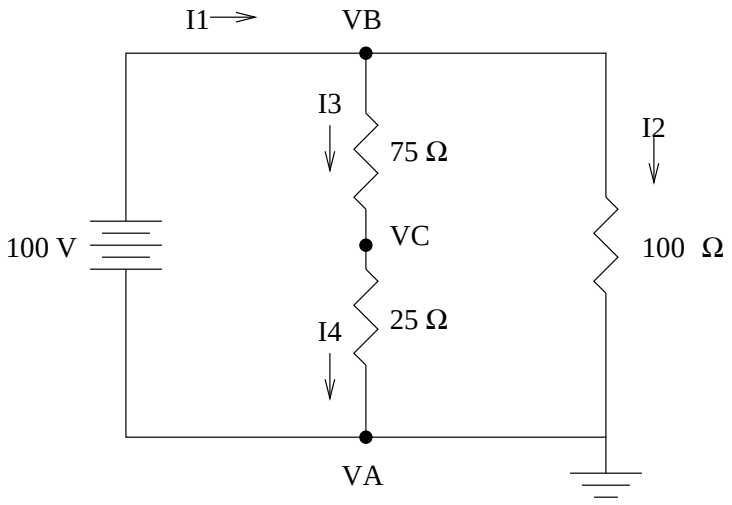


Figure 3.2: Circuit Analysis

Then we can write the general system above in the form $A \cdot X = B$. That is, if values $x_1 \ldots x_n$ satisfy the system of equations then the vector $\langle x_1 \ldots x_n \rangle$ will satisfy the matrix equation. For example, the particular system above can be written as the equation

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 0 & -1 & 3 \\ -1 & 2 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} w \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 2 \\ -1 \\ 2 \end{bmatrix}$$

In chapter 4, we will develop a mathematical theory that will allow us to categorize different types of systems of linear equations and their solutions. In particular, we will prove that a system of linear equations has either one solution, infinitely many solutions, or no solutions. In chapter 5, we will present an algorithm for solving systems of linear equations.

3.6.1 Applications of systems of linear equations

Many applications of all kinds involve solving systems of linear equations. Obviously we can take any of the above applications of matrix multiplication and turn them around to get a system of linear equations. For example, in the shopping application (4), we could ask, "Given a $m \times n$ price matrix P showing the prices of n items by at m stores, and a vector $\vec{c}$ of the cost of an unknown basket at each store, find a basket $\vec{x}$ satisfying $P\vec{x} = \vec{c}$." In the population transfer application (13) we could ask, "Given a distribution of population at the end of the year $\vec{v}$ and the transition matrix for the year M, find the distribution of population $\vec{x}$ at the start of the year"; this will be the solution to the problem $M\vec{x} = \vec{v}$.

Further applications follow; more will arise in the course of the book.

Application 17: Circuit analysis

A simple circuit of resistors and a power source, such as shown in figure 3.2, gives rise to a system of linear equation. The variables are the voltages at each node, the equations for the voltage source and for ground, the equations correspond to the resistor equation $V = I \cdot R$ (voltage difference equals

current times resistance), and Kirchoff's circuit law, stating that the total current flowing into a node is 0. (Kirchoff's voltage law, stating that the sum of the voltage drops around a cycle is 0, is built into our decision to represent the voltage at each node as a variable, rather than directly representing the voltage drop across each branch.) Applying these laws to the circuit in figure 3.2 we get the system of 8 equations in 7 unknowns:

$$V_A = 0$$

$$V_B - V_A = 100$$
$$V_B - V_A = 100 \cdot I_2$$
$$V_C - V_A = 75 \cdot I_3$$
$$V_B - V_C = 25 \cdot I_4$$
$$I_1 - I_2 - I_3 = 0$$
$$I_3 - I_4 = 0$$
$$I_4 + I_2 - I_1 = 0$$

Moving all the variable terms to the right and converting to matrix form, this becomes:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & -100 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & -75 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 & -25 \\ 0 & 0 & 0 & 1 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & -1 & 1 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} V_A \\ V_B \\ V_C \\ I_1 \\ I_2 \\ I_3 \\ I_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 100 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

The solution is $\langle 0, 100, 25, 2, 1, 1, 1 \rangle$.

Application 18: Temperature distribution

The distribution of temperature and other properties in a continuous material can be approximated by linear equations. For example suppose that you have a square bar of metal which is heated on one side by a hot-plate at $100°C$ and which on the other three sides borders the air at room temperature $20°C$. In a steady state, the temperature at each point is the average of the temperature at the neighboring points. This is made precise in the partial differential equation $\nabla^2 T = 0$, but it can be approximated by choosing a uniform grid of points inside the metal and asserting the relation at every point.[1]

If we choose a grid of nine interior points, as shown in figure 3.3 we get the following system of 9 equations in 9 unknowns:

$$T_1 = 1/4(20 + 20 + T_2 + T_4)$$
$$T_2 = 1/4(20 + T_1 + T_3 + T_5)$$
$$T_3 = 1/4(20 + 20 + T_2 + T_6)$$
$$T_4 = 1/4(20 + T_1 + T_5 + T_7)$$
$$T_5 = 1/4(T_2 + T_4 + T_6 + T_8)$$

[1] This example is from Philip Davis, *The Lore of Large Numbers,* Random House, 1960.

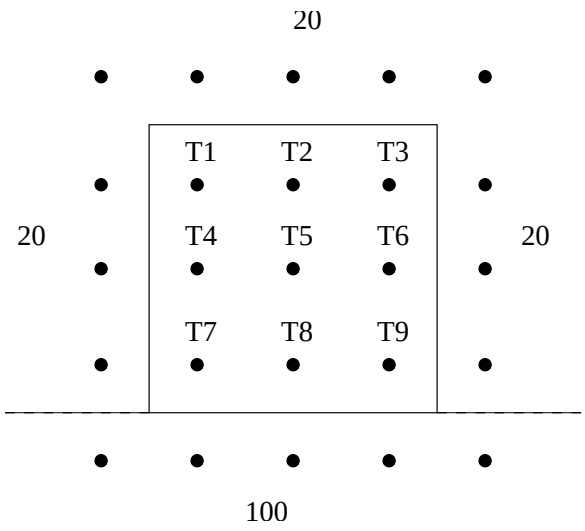


Figure 3.3: Heat distribution

$$T_6 = 1/4(20 + T_3 + T_5 + T_9)$$
$$T_7 = 1/4(20 + 100 + T_4 + T_8)$$
$$T_8 = 1/4(100 + T_5 + T_7 + T_9)$$
$$T_9 = 1/4(20 + 100 + T_6 + T_8)$$

This can be rewritten as the matrix equation

$$\begin{bmatrix} 1 & -1/4 & 0 & -1/4 & 0 & 0 & 0 & 0 & 0 \\ -1/4 & 1 & -1/4 & 0 & -1/4 & 0 & 0 & 0 & 0 \\ 0 & -1/4 & 1 & 0 & 0 & -1/4 & 0 & 0 & 0 \\ -1/4 & 0 & 0 & 1 & -1/4 & 0 & -1/4 & 0 & 0 \\ 0 & -1/4 & 0 & -1/4 & 1 & -1/4 & 0 & -1/4 & 0 \\ 0 & 0 & -1/4 & 0 & -1/4 & 1 & 0 & 0 & -1/4 \\ 0 & 0 & 0 & -1/4 & 0 & 0 & 1 & -1/4 & 0 \\ 0 & 0 & 0 & 0 & -1/4 & 0 & -1/4 & 1 & -1/4 \\ 0 & 0 & 0 & 0 & 0 & -1/4 & 0 & -1/4 & 1 \end{bmatrix} \cdot \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \\ T_7 \\ T_8 \\ T_9 \end{bmatrix} = \begin{bmatrix} 10 \\ 5 \\ 10 \\ 5 \\ 0 \\ 5 \\ 30 \\ 25 \\ 30 \end{bmatrix}$$

The solution is $\langle 25.71, 27.85, 25.71, 35, 40, 35, 54.29, 62.14, 54.29 \rangle$.

Application 19: Curve interpolation

Suppose you have a graph of q data points $\langle x_1, y_1 \rangle, \langle x_2, y_2 \rangle \ldots \langle x_q, y_q \rangle$, with independent variable x and dependent variable y, and you want to connect these with a smooth curve. This is known as *interpolating* a curve. One way to do this (not necessarily the best way) is to find a $q-1$ degree polynomial $y = t_{q-1}x^{q-1} + \ldots + t_1 x + t_0$ that fits the data. Finding the coefficients t_i can be viewed as solving a system of linear equations,[2] where the t_i are the variables, the coefficients are the powers of x_i and the constants are the y_i.

[2]There is also a simple closed formula for finding the coefficients of an interpolating polynomial.

For example, suppose you have the five data points, $\langle -3, 1\rangle, \langle -1, 0\rangle, \langle 0, 5\rangle, \langle 2, 0\rangle, \langle 4, 1\rangle$. We then have the following system of equations:

$$\begin{aligned} t_4(-3)^4 + t_3(-3)^3 + t_2(-3)^2 + t_1(3) + t_0 &= 1 \\ t_4(-1)^4 + t_3(-1)^3 + t_2(-1)^2 + t_1(1) + t_0 &= 0 \\ t_4(0)^4 + t_3(0)^3 + t_2(0)^2 + t_1(0) + t_0 &= 5 \\ t_4(2)^4 + t_3(2)^3 + t_2(2)^2 + t_1(2) + t_0 &= 0 \\ t_4(4)^4 + t_3(4)^3 + t_2(4)^2 + t_1(4) + t_0 &= 1 \end{aligned}$$

In matrix form:

$$\begin{bmatrix} 81 & -27 & 9 & -3 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 16 & 8 & 4 & 2 & 1 \\ 256 & 64 & 16 & 4 & 1 \end{bmatrix} \cdot \begin{bmatrix} t_4 \\ t_3 \\ t_2 \\ t_1 \\ t_0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 5 \\ 0 \\ 1 \end{bmatrix}$$

The solution is $\langle 13/60, -26/60, -163/60, 176/60, 5\rangle$.

This technique is not restricted to polynomials. Let $f_1 \ldots f_n$ be any set of n "basis" functions. (In the case of polynomials, these are the power functions $f_i(x) = x^i$.) If you wish to interpolate n data points by the linear sum $t_1 f_1(x) + \ldots + t_n f_n(x)$, then the weights t_i can be found by solving the associated system of linear equations $y_j = f_1(x_j)t_1 + \ldots + f_n(x_j)t_n$ for $j = 1 \ldots n$. (Depending on the functions, the system may have no solution or the solution may not be unique.) In this system, the coefficients are the values $f_i(x_j)$, the variables are the t_i, and the constant terms are the y_j

For instance, suppose that we use the five basis functions 1, $\sin(\pi x/2)$, $\sin(\pi x/4)$, $\cos(\pi x/2)$, $\cos(\pi x/6)$. Then the coefficients of the curve that interpolates the same set of data points satisfy the system

$$\begin{bmatrix} 1 & 1 & -1/\sqrt{2} & 0 & 0 \\ 1 & -1 & -1/\sqrt{2} & 0 & \sqrt{3}/2 \\ 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & -1 & 0.5 \\ 1 & 0 & 0 & 1 & -0.5 \end{bmatrix} \cdot \begin{bmatrix} t_4 \\ t_3 \\ t_2 \\ t_1 \\ t_0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 5 \\ 0 \\ 1 \end{bmatrix}$$

The solution is $\langle -0.217, 1.6547, 0.9566, 2.3116, 2.6667\rangle$.

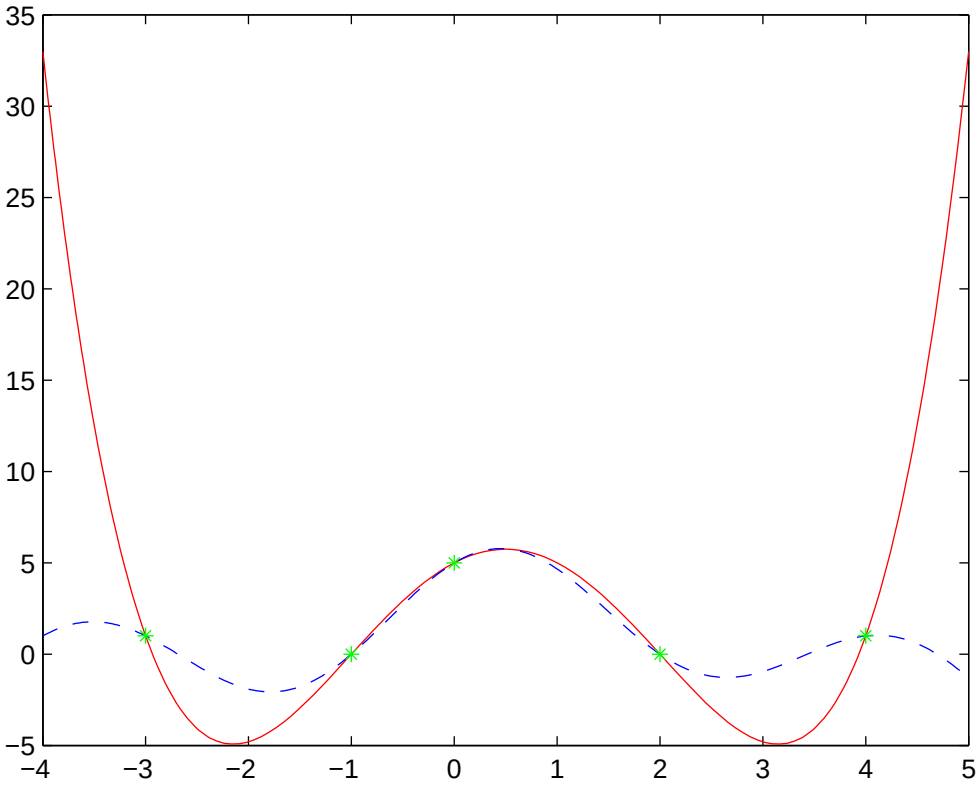
The two interpolations are shown in figure 3.4

3.7 Matrix multiplication

In view of theorem 3.1, we can now look at basic operations on linear transformations, and ask how these work out in terms of the corresponding matrices. In this section, we will look at three operators: multiplication of a transformation by a scalar and addition of two transformation, which are easy, and the *composition* of two transformations, which requires some work. The final important operator is the *inverse* of a transformation; that is much more complicated and will be dealt with in section 5.3.

First, two easy definitions. If $f(\vec{x})$ and $g(\vec{x})$ are linear transformations from $\mathbb{R}^n$ to $\mathbb{R}^m$ and a is a scalar, then we define the transformation $a \cdot f$ by the equation $(a \cdot f)(\vec{x}) = a \cdot f(\vec{x})$ and we define the transformation $f + g$ by the equation $(f + g)(\vec{x}) = f(\vec{x}) + g(\vec{x})$. It is easy to check that:

- $a \cdot f$ and $f + g$ are both linear transformation.



The polynomial interpolation is the solid red line.
The sinusoidal interpolation is the dashed blue line.

Figure 3.4: Interpolation

- Let F be the matrix corresponding to f and let G be the matrix corresponding to g. Then $a \cdot F$ corresponds to $a \cdot f$ and $F + G$ corresponds to $f + g$.

We now turn to composition, which is not so simple. Suppose that $f(\vec{x})$ is a linear transformation from $\mathbb{R}^n$ to $\mathbb{R}^m$ and that $g(\vec{x})$ is a linear transformation from $\mathbb{R}^m$ to $\mathbb{R}^p$. Then the composition $g \circ f$ is the function from $\mathbb{R}^n$ to $\mathbb{R}^p$ defined as $(g \circ f)(\vec{x}) = g(f(\vec{x}))$. It is easily to show that $g \circ f$ is likewise a linear transformation, as follows:

- $(g \circ f)(a \cdot \vec{x}) =$ (by definition)
  $g(f(a \cdot \vec{x})) =$ (since f is linear)
  $g(a \cdot f(\vec{x})) =$ (since g is linear)
  $a \cdot g(f(\vec{x})) = a \cdot (g \circ f)(\vec{x})$ (by definition).
- $(g \circ f)(\vec{x} + \vec{y}) =$ (by definition)
  $g(f(\vec{x} + \vec{y})) =$ (since f is linear)
  $g(f(\vec{x}) + f(\vec{y})) =$ (since g is linear)
  $g(f(\vec{x})) + g(f(\vec{y})) = (g \circ f)(\vec{x}) + (g \circ f)(\vec{y})$ (by definition).

Therefore by theorem 3.1, there is a matrix M corresponding to the transformation $g \circ f$. The question is, how is M related to G and F, the matrices corresponding to functions f and g?

The answer is that M is the *matrix product* $G \cdot F$. We can determine how this product is computed by studying how it operates on a sample vector. To avoid giving ourselves the headache brought on by too many subscripts and summation signs, we will work through an example with specific numbers where $n = 3$, $m = 2$, $p = 3$. Let G, F, and $\vec{v}$ be the following matrices:

$$G = \begin{bmatrix} 67 & 68 \\ 77 & 78 \\ 87 & 88 \end{bmatrix} \qquad F = \begin{bmatrix} 31 & 32 & 33 \\ 41 & 42 & 43 \end{bmatrix} \qquad \vec{v} = \begin{bmatrix} 10 \\ 11 \\ 12 \end{bmatrix}$$

Let f and g be the transformations corresponding to F and G, and let H be the matrix corresponding to $g \circ f$. Then we have

$$H \cdot \vec{v} = (g \circ f)(\vec{v}) = g(f(\vec{v})) = G \cdot (F \cdot \vec{v}) =$$

$$\begin{bmatrix} 67 & 68 \\ 77 & 78 \\ 87 & 88 \end{bmatrix} \cdot \left(\begin{bmatrix} 31 & 32 & 33 \\ 41 & 42 & 43 \end{bmatrix} \cdot \begin{bmatrix} 10 \\ 11 \\ 12 \end{bmatrix} \right) = \begin{bmatrix} 67 & 68 \\ 77 & 78 \\ 87 & 88 \end{bmatrix} \cdot \begin{bmatrix} 31 \cdot 10 + 32 \cdot 11 + 33 \cdot 12 \\ 41 \cdot 10 + 42 \cdot 11 + 43 \cdot 12 \end{bmatrix} =$$

$$\begin{bmatrix} 67 \cdot (31 \cdot 10 + 32 \cdot 11 + 33 \cdot 12) + 68 \cdot (41 \cdot 10 + 42 \cdot 11 + 43 \cdot 12) \\ 77 \cdot (31 \cdot 10 + 32 \cdot 11 + 33 \cdot 12) + 78 \cdot (41 \cdot 10 + 42 \cdot 11 + 43 \cdot 12) \\ 87 \cdot (31 \cdot 10 + 32 \cdot 11 + 33 \cdot 12) + 88 \cdot (41 \cdot 10 + 42 \cdot 11 + 43 \cdot 12) \end{bmatrix} =$$

$$\begin{bmatrix} (67 \cdot 31 + 68 \cdot 41) \cdot 10 + (67 \cdot 32 + 68 \cdot 42) \cdot 11 + (67 \cdot 33 + 68 \cdot 43) \cdot 12 \\ (77 \cdot 31 + 78 \cdot 41) \cdot 10 + (77 \cdot 32 + 78 \cdot 42) \cdot 11 + (77 \cdot 33 + 78 \cdot 43) \cdot 12 \\ (87 \cdot 31 + 88 \cdot 41) \cdot 10 + (87 \cdot 32 + 88 \cdot 42) \cdot 11 + (87 \cdot 33 + 88 \cdot 43) \cdot 12 \end{bmatrix} =$$

$$\begin{bmatrix} 67 \cdot 31 + 68 \cdot 41 & 67 \cdot 32 + 68 \cdot 42 & 67 \cdot 33 + 68 \cdot 43 \\ 77 \cdot 31 + 78 \cdot 41 & 77 \cdot 32 + 78 \cdot 42 & 77 \cdot 33 + 78 \cdot 43 \\ 87 \cdot 31 + 88 \cdot 41 & 87 \cdot 32 + 88 \cdot 42 & 87 \cdot 33 + 88 \cdot 43 \end{bmatrix} \cdot \begin{bmatrix} 10 \\ 11 \\ 12 \end{bmatrix}$$

Therefore

$$G \cdot F = H = \begin{bmatrix} 67 \cdot 31 + 68 \cdot 41 & 67 \cdot 32 + 68 \cdot 42 & 67 \cdot 33 + 68 \cdot 43 \\ 77 \cdot 31 + 78 \cdot 41 & 77 \cdot 32 + 78 \cdot 42 & 77 \cdot 33 + 78 \cdot 43 \\ 87 \cdot 31 + 88 \cdot 41 & 87 \cdot 32 + 88 \cdot 42 & 87 \cdot 33 + 88 \cdot 43 \end{bmatrix}$$

Each element of H, $H[i, j]$ corresponds to the dot product of the row $G[i, :]$ with the column $F[:, j]$. The same thing works in the same way for any matrices F and G.

Definition 3.2. *Let F be a $m \times n$ matrix and let G be a $p \times m$ matrix. The product $G \cdot F$ is the $p \times n$ matrix defined by the rule*

$$(G \cdot F)[i,j] = G[i,:] \bullet F[:,j] = \sum_{k=1}^{m} G[i,k] \cdot F[k,j]$$

The matrix product $G \cdot F$ is defined only if the number of columns in G is equal to the number of rows in F.

Theorem 3.2. *Let f be a linear transformation from $\mathbb{R}^m$ to $\mathbb{R}^k$, let g be a linear transformation from $\mathbb{R}^k$ to $\mathbb{R}^m$, and let F and G be the corresponding matrices. Then the product $G \cdot F$ is the matrix corresponding to the composition $g \circ f$.*

In manually computing the product of two matrices $G \cdot F$, again you use the two hands method: The left hand moves left to right along the ith row G, the right hand moves top to bottom down the jth column of F, you multiply the two numbers and add them to a running total, and the final sum is the $[i,j]$th entry in $G \cdot F$.

A particular significant linear transformation is the *identity* on n-dimensional vectors; that is, the function i defined by $i(\vec{v}) = \vec{v}$ for all n-dimensional vectors $\vec{v}$. It is easy to show that the corresponding matrix, known as the identity matrix and denoted I_n, is the $n \times n$ matrix with 1's on the diagonal from the upper left to the lower right and 0's everywhere else. For example,

$$I_6 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

3.7.1 Applications of matrix multiplication

Example: A simple application of matrix multiplication is to compute all pairs of dot products of one collection of vectors by another collection of vectors. In the shopping application, for instance suppose there are m stores, p items, and n shopping baskets. Let P be the $m \times p$ matrix whose rows are price vectors; that is $P[i,k]$ is the price of item k in shop i. Let B be the $p \times n$ matrix whose columns are baskets; that is, $B[k,j]$ is the number of item k in basket j. Then the product $P \cdot B$ is the $m \times p$ matrix showing the price of each basket at each store; that is, $(P \cdot B)[i,j]$ is the price of basket j at store i.

Example: As an example of composition of transformations, suppose that a customer Joe is shopping for the ingredients of a number of recipes for a party. Suppose that there are n recipes, p types of groceries, m stores. Let $\vec{d}$ be the "party vector" showing the number of servings of each dish that Joe is planning to make. Let R be the matrix of recipe ingredients; that is, $R[k,j]$ is the amount of ingredient k needed for one serving of recipe j. Then $R \cdot \vec{d}$ is the basket vector; that is, $(R \cdot \vec{d})[k]$ is the number of units of ingredient k that Joe needs to buy. Thus, multiplication by R corresponds to a linear transformation mapping a party vector to a shopping basket. Let P be the price matrix; that is, $P[i,k]$ is price of item k at store i. Then, for any basket $\vec{b}$, $P \cdot \vec{b}$ is the vector showing the cost of basket $\vec{b}$ at each store. Thus, P is a transformation from basket vectors to vectors of cost by store. Therefore, the product $P \cdot R$ is the transformation from party vectors to the vector showing

the cost of the entire party by store. That is, if $\vec{p} = (P \cdot R) \cdot \vec{d} = P \cdot (R \cdot \vec{d})$, then $\vec{p}[i]$ is the price of buying all the ingredients for the party at store i.

Example: Combining applications 14 and 15 of signal processing, if we want to carry out a smoothing operation and then a time shift, the combined operation corresponds to multiplication by the product $H \cdot M$ where M is the matrix for the smoothing and H is the matrix for the time shift.

Example: In application 13 of population transfer, suppose that A, B, and C are the matrices of population transfer in years 1, 2, and 3 respectively, and $\vec{v}$ is the population vector at the start of year 1. Then $A\vec{v}$ is the population vector at the end of year 1; $B \cdot (A\vec{v}) = (B \cdot A)\vec{v}$ is the population vector at the end of year 2; and $C \cdot ((B \cdot A) \cdot \vec{v}) = (C \cdot B \cdot A) \cdot \vec{v}$ is the population vector at the end of year 3. Thus $B \cdot A$ is the transfer matrix for years 1 and 2 combined and $C \cdot B \cdot A$ is the transfer matrix for years 1, 2, and 3 combined.

Example: In application 16 of partial derivatives, it is easily shown that if $\mathbf{F}$ is a differentiable function from $\mathbb{R}^n$ to $\mathbb{R}^m$ and $\mathbf{G}$ is a differentiable function from $\mathbb{R}^m$ to $\mathbb{R}^p$ then the Jacobian of the composition $J(\mathbf{G} \circ \mathbf{F}) = J(\mathbf{G}) \cdot J(\mathbf{F})$.

3.8 Vectors as matrices

The operation of multiplying $m \times n$ matrix M times n-dimensional vector $\vec{v}$ can be viewed as a special case of multiplying two matrices if $\vec{v}$ is associated with the $n \times 1$ matrix V, consisting of a single column. The operation of computing the dot product of two n-dimensional vectors $\vec{u} \bullet \vec{v}$ can be viewed as a special case of multiplying two matrices if $\vec{u}$ is associated with the $1 \times n$ matrix U, consisting of a single row and $\vec{v}$ is associated with the $n \times 1$ matrix V, consisting of a single column.

Thus, sometimes it is convenient to associate vectors with rows, and sometimes it is convenient to associate them with columns, and you may have to do both in the same equation. In the mathematical literature, vectors are more often associated with $n \times 1$ matrices (i.e. column vectors), so one writes the product of M by $\vec{v}$ as $M \cdot \vec{v}$, and the dot product of $\vec{u}$ and $\vec{v}$ as $\vec{u}^T \cdot \vec{v}$. (The notation $\vec{u}^T \cdot \vec{v}$ is sometimes used for the dot product even in contexts where there are no matrices involved; I prefer $\vec{u} \bullet \vec{v}$ in such cases.) MATLAB tries to be even-handed, but when forced to choose, opts for row vectors. Thus, as discussed in section 2.5, MATLAB functions with vector arguments such as `dot(X,Y)` or `norm(X)` generally work with either row or column vectors; built-in functions that return vectors such as `size(A)` generally return row rather than column vectors.

If U is a $1 \times m$ row vector and M is an $m \times n$ matrix, then the product $U \cdot M$ is a $1 \times n$ vector; this is sometimes useful. If U is a $1 \times n$ row vector and V is an $n \times 1$ column matrix, then the product $V \cdot U$ is an $n \times n$ matrix, consisting of all the products of an element of V times an element of U.

3.9 Algebraic properties of matrix multiplication

The following basic algebraic properties of matrix multiplication are important. In the following, A and B are $m \times n$ matrices; C and D are $n \times p$ matrices; E is a $p \times q$ matrix; a is a scalar. I_n is the $n \times n$ identity matrix

1. $A \cdot (C \cdot E) = (A \cdot C) \cdot E$. (Associativity)
2. $A \cdot (C + D) = (A \cdot C) + (A \cdot D)$. (Right distributivity).
3. $(A + B) \cdot C = (A \cdot C) + (B \cdot C)$. (Left distributivity).
4. $a \cdot (A \cdot B) = (a \cdot A) \cdot B = A \cdot (a \cdot B)$.
5. $A \cdot I_n = A$. (Right identity)

6. $I_n \cdot C = C$. (Left identity)
7. $(A \cdot B)^T = B^T \cdot A^T$.

All of these can be proven, without difficulty though somewhat drearily, from definition 3.2 for matrix multiplication. For (1-6) however, it is even easier, and much more enlightening, to derive them using the correspondence with linear transformation. (It is not possible to derive (7) this way, because, as mentioned above, transpose does not correspond to anything simple in the world of linear transformations.)

For instance, to establish rule (2), let c and d be linear transformations from $\mathbb{R}^p$ to $\mathbb{R}^n$; and let a be a linear transformation from $\mathbb{R}^n$ to $\mathbb{R}^m$. Then we have

$(a \circ (c + d))(\vec{v}) =$ (by definition of composition)
$a((c + d)(\vec{v})) =$ (by definition of $c + d$)
$a(c(\vec{v}) + d(\vec{v})) =$ (by linearity of a)
$a(c(\vec{v})) + a(d(\vec{v})) =$ (by definition of composition)
$(a \circ c)(\vec{v}) + (a \circ d)(\vec{v}) =$ (by definition of $(a \circ c) + (a \circ d)$)
$((a \circ c) + (a \circ d))(\vec{v})$.

Since $a \circ (c + d)$ corresponds to $A(C + D)$ and $(a \circ c) + (a \circ d)$ corresponds to $AC + AD$, we have $A(C + D) = AC + AD$.

VERY IMPORTANT: Matrix multiplication is not commutative. That is, $A \cdot B$ is not in general equal to $B \cdot A$.

In particular let A is a $m \times n$ matrix and B is a $p \times q$ matrix, then

- AB is defined only if $n = p$ and BA is defined only if $q = m$.
- Suppose that $n = p$ and $q = m$, so that both products are defined. Then AB is an $m \times m$ matrix and BA is an $n \times n$ matrix, so that the two products are the same shape only if $n = m$.
- Even if $m = n = p = q$, so that both products are defined and have the same shape, still in most cases $AB \neq BA$. For example:

$$\text{Let } A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \text{ and let } B = \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix}$$

Then

$$AB = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \cdot \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix} = \begin{bmatrix} 19 & 22 \\ 43 & 50 \end{bmatrix} \text{ but } BA = \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix} \cdot \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} = \begin{bmatrix} 23 & 34 \\ 31 & 46 \end{bmatrix}$$

3.9.1 Matrix exponentiation

If A is a square $n \times n$ matrix, then the product $A \cdot A$ is defined and is likewise an $n \times n$ matrix. Therefore, one can continue multiplying by A and multiply A by itself k times. The product $A \cdot A \cdot \ldots \cdot A$ (k times) is, naturally, denoted A^k.

For example, suppose that in the population transition example (application 13) the transition matrix M is constant year after year. Then after k years, the population vector will be $M^k \cdot \vec{v}$ where $\vec{v}$ is the population vector at the start.

Another example: Consider the Fibonacci series, 1, 1, 2, 3, 5, 8, ... defined by the recurrence $F(1) = 1$, $F(2) = 1$, $F(i) = F(i - 1) + F(i - 2)$ for $n > 2$. This can be characterized in terms of

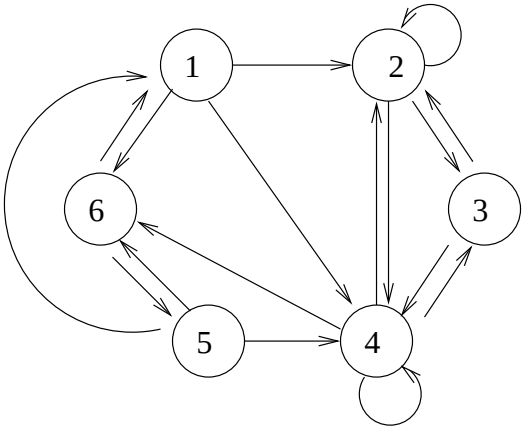


Figure 3.5: Directed graph

matrix exponentiation as follows:[3] Consider the sequence of vectors $\vec{V}(1) = \langle 1, 1\rangle$, $\vec{V}(2) = \langle 1, 2\rangle$, $\vec{V}(3) = \langle 2, 3\rangle$, and so on, where $\vec{V}(i)$ is the 2-dimensional vector $\langle F(i), F(i+1)\rangle$. Then the recurrence condition above can be expressed in the formula $\vec{V}(i+1) = M \cdot \vec{V}(i)$, where

$$M = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$$

Therefore $\vec{V}(i) = M^{i-1}\vec{V}(1)$.

Application 20: Paths in a directed graph Let matrix A be the adjacency matrix for graph G; that is, $A[I, J] = 1$ if there is an edge from vertex I to vertex J in G and 0 otherwise. For example, the adjacency matrix for the graph in figure 3.5 is

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

Thus, for example, $A[1, 4] = 1$ because there is an arc from vertex 1 to vertex 4.

Now, there is a path of length 2, $U \rightarrow V \rightarrow W$ in G just if $A[U, V]$ and $A[V, W]$ are both 1; that is, if $A[U, V] \cdot A[V, W] = 1$. Therefore, the number of paths of length 2 from U to W is equal to $\sum_{V=1}^{N} A[U, V] \cdot A[V, W] = A^2[U, W]$. That is, the matrix A^2 is the matrix such that for all U and W, $A^2[U, W]$ is the number of paths of length 2 from U to W.

In fact in general, for any power k, $A^k[U, W]$ is the number of paths from U to W of length k. Proof by induction: Suppose this is true for $k-1$. Now consider the paths of length k from U to W where the second vertex is V. If there is an arc from U to V then the number of such paths is equal to the number of paths of length $k-1$ from V to W, which by induction is $A^{k-1}[V, W]$. If there is no arc from U to V, then the number of such paths is 0. In either case, the number of such paths is $A[U, V] \cdot A^{k-1}[V, W]$. But the total of paths of length k from U to W is the sum over all vertices V of the paths whose second vertex is V; that is, $\sum_V A[U, V] \cdot A^{k-1}[V, W] = (A \cdot A^{k-1})[U, W] = A^k[U, W]$.

[3] This is not an effective way of computing Fibonacci numbers; just an interesting way of characterizing them.

3.10 Matrices in MATLAB

Inputting matrices. Items in a row are separated by commas or space bar; rows are separated by semi-colon or line breaks.

```
>> a=[11,12,13; 14,15,16]
a =
    11    12    13
    14    15    16

>> b=[
1 2 3
4 5 6]
b =
     1     2     3
     4     5     6

>> % Identity matrix (square)
>> eye(5)
ans =
     1     0     0     0     0
     0     1     0     0     0
     0     0     1     0     0
     0     0     0     1     0
     0     0     0     0     1

>> % Rectangular identity matrix
>> eye(5,3)
ans =
     1     0     0
     0     1     0
     0     0     1
     0     0     0
     0     0     0

>> % Square zero matrix
>> zeros(4)
ans =
     0     0     0     0
     0     0     0     0
     0     0     0     0
     0     0     0     0


>> % Rectangular zero matrix
>> zeros(2,4)
ans =
     0     0     0     0
     0     0     0     0

>> % Square matrix of 1's
```

```
>> ones(5)
ans =
     1     1     1     1     1
     1     1     1     1     1
     1     1     1     1     1
     1     1     1     1     1
     1     1     1     1     1

>> % Diagonal matrix
>> diag([1,4,9,16])
ans =
     1     0     0     0
     0     4     0     0
     0     0     9     0
     0     0     0    16
```

Indexing into matrices. Extracting submatrices.

```
>> a
a =
    11    12    13
    14    15    16

>> a(1,2)
ans =
    12

>> a(2,3)
ans =
    16

>> a(2,3)=20
a =
    11    12    13
    14    15    20

>> a(3,5)=25
a =
    11    12    13     0     0
    14    15    20     0     0
     0     0     0     0    25

>> a(2,:)
ans =
    14    15    20     0     0

>> a(:,3)
ans =
    13
    20
     0
```

```
>> a(2:3,2:4)
ans =
    15    20     0
     0     0     0
```

Operations on matrices

```
>> a=[1,1,2; 3,4,5]
a =
     1     1     2
     3     4     5

>> b=[1,0,-1; 2,2,1]
b =
     1     0    -1
     2     2     1

>> c=[0,1;2,2;-1,0]
c =
     0     1
     2     2
    -1     0

>> a+b
ans =
     2     1     1
     5     6     6

>> a*c
ans =
     0     3
     3    11

>> c*a
ans =
     3     4     5
     8    10    14
    -1    -1    -2

>> % Transpose
>> a'
ans =
     1     3
     1     4
     2     5

>> v=[1,2,3]
v =
     1     2     3

>> a*v
ans =
```

```
     9
    26

> size(a)
ans =
     2     3

>> size(v)
ans =
     1     3

>> % Element by element multiplication
>> a.*b
ans =
     1     0    -2
     6     8     5

>> % Scalar operations
>> 2*a
ans =
     2     2     4
     6     8    10

>> a+2
ans =
     3     3     4
     5     6     7

>> % Matrix exponentiation
>> p=a(:,1:2)
p =
     1     1
     3     4

>> p^2
ans =
     4     5
    15    19

>> p^5
ans =
         436         551
        1653        2089

>> f=[0,1;1,1]
f =
     0     1
     1     1

>> v=[1,1]'
v =
```

```
     1
     1

>> f*v
ans =
     1
     2

>> f^2*v
ans =
     2
     3

>> f^10*v
ans =
    89
   144

>> f^10
ans =
    34    55
    55    89
```

3.10.1 Sparse matrices

Sparse matrices can be created with dimensions up to a large integer size.[4] The function "sparse" with a variety of types of arguments creates a sparse matrix. Many standard operations on full matrices can be applied to sparse matrices; some, such as computing rank, require specialized functions. The function `full(s)` converts a sparse matrix `s` to a full matrix.

```
% If A is a full matrix, then sparse(A) converts it to a sparse matrix
>> s=sparse(eye(6))
s =
   (1,1)        1
   (2,2)        1
   (3,3)        1
   (4,4)        1
   (5,5)        1
   (6,6)        1

% Note that a sparse matrix prints out by printing all the non-zero values
% with indices

% Indexing into a sparse matrix.
>> s(2,3) = 6
s =
   (1,1)        1
```

[4] According to the documentation, the dimension can be up to the maximum integer $2^{31} - 1$, but, at least with the version of MATLAB that I have been running, I have found that one can get errors if the size is more than about 500,000,000. Moreover, the behavior is erratic around that value; the call `sparse(498182000)` sometimes succeeds and sometimes gives an error.

```
   (2,2)        1
   (2,3)        6
   (3,3)        1
   (4,4)        1
   (5,5)        1
   (6,6)        1

% Multiplying sparse matrices
>> s*s
ans =
   (1,1)        1
   (2,2)        1
   (2,3)       12
   (3,3)        1
   (4,4)        1
   (5,5)        1
   (6,6)        1

% Other operations
>> size(s)
ans =
     6     6

% Converting a sparse matrix to a full matrix
>> full(s)
ans =
     1     0     0     0     0     0
     0     1     6     0     0     0
     0     0     1     0     0     0
     0     0     0     1     0     0
     0     0     0     0     1     0
     0     0     0     0     0     1

% Other ways to create sparse matrices
% sparse(m,n) creates a m*n sparse 0 matrix

>> s=sparse(3,5)
s =
   All zero sparse: 3-by-5
>> s(1,3)=5
s =
   (1,3)        5

% sparse(i,j,v,m,n,maxnz): i, j, v are vectors of equal length
% creates an m*n sparse matrix S such that S(i(k), j(k)) = v(k)
% maxnz is an upper bound on the number of non-zero elements in this call

>> s=sparse([1,2,3], [1,5,4], [3.1, 2.6, 5.0], 7, 6, 10)
s =
   (1,1)       3.1000
   (3,4)       5.0000
```

```
   (2,5)       2.6000

% speye(n) creates the sparse n x n identity matrix

>> speye(6)
ans =
   (1,1)        1
   (2,2)        1
   (3,3)        1
   (4,4)        1
   (5,5)        1
   (6,6)        1
```

3.10.2 Cell arrays

Cell arrays are heterogeneous arrays; that is, unlike regular arrays, the entities in a single cell array may vary in type and size. They are created and indexed using curly brackets. They are useful in creating "ragged arrays" such as collections of vectors, strings, or matrices of different kinds.

```
>> c={1, [1,2], 'Do-re-mi', [1,2,3;4,5,6]}
c =
    [1]    [1x2 double]    'Do-re-mi'    [2x3 double]

>> c{3}
ans =
Do-re-mi

>> text={'Fourscore', 'and', 'seven', 'years', 'ago'}
text =
    'Fourscore'    'and'    'seven'    'years'    'ago'

>> text{4}
ans =
years

>> m={eye(1),eye(2),eye(3),eye(4)}
m =
    [1]    [2x2 double]    [3x3 double]    [4x4 double]

>> m{2}
ans =
     1     0
     0     1
```

Exercises

Exercise 3.1

$$\begin{bmatrix} 2 & -1 & 1 \\ 1 & 3 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 3 & -2 \\ 1 & 2 & 3 \end{bmatrix}$$

Exercise 3.2

$$\begin{bmatrix} 2 & -1 & 1 & 0 \\ 1 & 3 & 1 & -1 \\ -2 & 1 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ -2 \\ 2 \\ 1 \end{bmatrix}$$

Exercise 3.3

$$\begin{bmatrix} 1 & -2 & 1 \end{bmatrix} \cdot \begin{bmatrix} 2 & -1 & 1 & 0 \\ 1 & 3 & 1 & -1 \\ -2 & 1 & 0 & 1 \end{bmatrix}$$

Exercise 3.4

$$\begin{bmatrix} 2 & -1 & 1 & 0 \\ 1 & 3 & 1 & -1 \\ -2 & 1 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 2 \\ -2 & 0 \\ 2 & -1 \\ 1 & 1 \end{bmatrix}$$

Exercise 3.5

Let

$$A = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix} \qquad B = \begin{bmatrix} 3 & 1 & 2 \end{bmatrix} \qquad C = \begin{bmatrix} 2 \\ -1 \\ 2 \end{bmatrix}$$

Compute the product of these three matrices, first as $(A \cdot B) \cdot C$ and second as $A \cdot (B \cdot C)$. Which method involves fewer integer multiplications?

Exercise 3.6

A *permutation matrix* is a square matrix such that each row and each column has one entry of 1 and the rest 0. For instance, the matrix

$$M = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

is a 6×6 permutation matrix.

A. Let V be the row vector $[1, 2, 3, 4, 5, 6]$. What is $V \cdot M$? What is $M \cdot V^T$?

B. Let U be the row vector $[4, 5, 6, 3, 2, 1]$. Construct a permutation matrix such that $V \cdot M = U$. Construct a permutation matrix such that $U \cdot M = V$. What do you notice about these two matrices?

Exercise 3.7

In the graph of figure 3.5, section 3.9.1,

A. Find the number of paths of length 6 from A to F.

B. Draw a plot of the number of all paths in the graph of length K, as a function of K, for $K = 1 \ldots 10$.

Problems

Problem 3.1

A. Prove each of axioms 1-7 p. 56 directly from the numerical definition of matrix multiplication.

B. Prove each of axioms 1-6, except (2), using an argument based on linear transformations, analogous to the argument for axiom (2) given in the text.

Problem 3.2

What is the advantage of using the function `speye(N)` over writing the expression `sparse(eye(N))`?

Problem 3.3

Let M be an $n \times n$ permutation matrix as defined in exercise 3.6. Prove that $M \cdot M^T = I_n$. (Hint: What is the dot product of a row of M with a column of M^T?).

Problem 3.4

Show that none of the operations sort($\vec{v}$), max($\vec{v}$) or product($\vec{v}$) is a linear transformation.

Problem 3.5

A) Prove that the operation of taking the transpose of a matrix does not correspond to matrix multiplication. That is, there does not exists an $n \times n$ matrix M such that, for every $n \times n$ matrix A, $M \cdot A = A^T$. Hint: Use the fact that, for any two matrices U, V and any index i, $U \cdot (V[:, i]) = (U \cdot V)[:, i]$

Note that, if A is a pixel array, then A^T is the reflection of the image across the main diagonal; thus, this illustrates that geometric transformations on pixel arrays do not correspond to matrix multiplication. This will be discussed further in section 6.4.8.

B) (Tricky). However, transpose is a linear operator. That is, suppose we define a function $\Phi(A) = A^T$. Then Φ satisfies the equations

$$\Phi(A + B) = \Phi(A) + \Phi(B)$$
$$\Phi(c \cdot A) = c \cdot \Phi(A).$$

But we proved in theorem 3.1 that every linear operator *does* correspond to matrix multiplication. Resolve the apparent contradiction.

Problem 3.6

A square matrix A is *nilpotent* if $A^p = 0$ for some power p.

A. Prove that an adjacency matrix A for graph G is nilpotent if and only if G is acyclic (a DAG).

B. Consider the smallest value of p for which $A^p = 0$. What is the significance of p in terms of the graph G?

Programming Assignments

Assignment 3.1: Evaluating a linear classifier

Consider a classification problem of the following kind: You are given n numeric features of an entity and you want to predict whether or not the entity belongs to a specific category. For example, based on measurable geometric features, is a given image a picture of a camel? Based on test results, does a patient have diabetes? Based on financial data, is a prospective business a good investment?

A *linear classifier* consists of a n-dimensional weight vector $\vec{W}$ and and a numeric threshold T. The classifier predicts that a given entity $\vec{X}$ belongs to the category just if $\vec{W} \bullet \vec{X} \geq T$.

Suppose, now, that you have a data set consisting of collection D of m entities together with the associated correct labels $\vec{L}$. Specifically, D is an $m \times n$ matrix, where each row is the feature vector for one entity. Vector $\vec{L}$ is a m-dimensional column vector, where $\vec{L}[i] = 1$ if the ith entity is in the category and 0 otherwise.

There are a number of different ways of evaluating how well a given classifier fits a given labelled data set. The simplest is the *overall accuracy* which is just the fraction of the instances in the data set where the classifier gets the right answer.

Overall accuracy, however, is often a very unhelpful measure. Suppose you are trying to locate pictures of camels in a large collection of images collected across the internet. Then, since images of camels constitutes only a very small fraction of the collection, you can achieve a high degree of overall accuracy simply by rejecting all the images. Clearly, this is not a useful retrieval engine.

In this kind of case, the most commonly used measures are *precision/recall*. Let C be the set of entities which are actually in the category (i.e. labelled so by $\vec{L}$); let R be the set of entities which the classifier predicts are in the category; and let $Q = C \cap R$. Then precision is defined as $|Q|/|R|$ and recall is defined as $|Q|/|C|$. In the camel example, the precision is the fraction of images that are actually camels, out of all the images that the classifier identifies as camels; and the recall is the fraction of the images of camels in the collection that the classifier acccepts as camels.

A. Write a MATLAB function `evaluate(D,L,W,T)` which takes as arguments D, L, W, and T, as described above, and which returns the overall accuracy, the precision, and the recall.

For example let $m = 6$, $n = 4$,

$$D = \begin{bmatrix} 1 & 1 & 0 & 4 \\ 2 & 0 & 1 & 1 \\ 2 & 3 & 0 & 0 \\ 0 & 2 & 3 & 1 \\ 4 & 0 & 2 & 0 \\ 3 & 0 & 1 & 3 \end{bmatrix} \qquad L = \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad W = \begin{bmatrix} 1 \\ 2 \\ 1 \\ 2 \end{bmatrix} \qquad T = 9$$

Then the classifications returned by the classifier are $[1, 0, 0, 1, 0, 1]$; the first, third, and fifth rows are correctly classified and the rest are misclassified. Thus, the accuracy is $3/6 = 0.5$. The precision is $1/3$; of the three instances identified by the classifier, only one is correct. The recall is $1/2$; of the two actual instances of the category, one is identified by the classifier.

B. Write a function `evaluate2(D,L,W,T)`. Here the input arguments D and L are as in part (A). W and T, however, represent a collection of q classifiers. W is a $n \times q$ matrix; T is a q-dimensional vector. For $j = 1 \ldots q$, the column W[;j] and the value T[j] are the weight vector and threshold of a classifier. `E=evaluate2(D,L,W,T)` returns a $3 \times q$ matrix, where, for $j = 1 \ldots q$, E[1,j], E[2,j] and E[3,j] are respectively the accuracy, precision, and recall of the jth classifier.

For example, let D and L be as in part (A). Let $q = 2$ and let

$$W = \begin{bmatrix} 1 & 0 \\ 2 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix} \qquad T = [9, 2]$$

Then evaluate2(D,L,W,T) =

$$\begin{bmatrix} 0.5 & 0.3333 \\ 0.6667 & 0.5 \\ 0.5 & 0.5 \end{bmatrix}$$

Assignment 3.2

Write a function `TotalPaths(A)` which takes as argument an adjacency matrix `A` for graph `G` and returns the total number of different paths of any length in `G`, if this is finite, or `Inf`, if there are infinitely many paths. Note: in the latter case it should *return* `Inf`, it should *not* go into an infinite loop.

Hint: It may be useful to do problem 3.6 first.

Assignment 3.3

The transition matrix model discussed in application 13 can also be used to model diffusion of unevenly distributed material in space over time. As in the discussion of temperature distribution (application 18), divide space up into a grid of points numbered $1 \ldots N$. Let $\vec{v}_T[I]$ be the amount of material I at time T. Let $D[I, J]$ be a transition matrix that expresses the fraction of the material at J that flows to I in each unit of time. In particular, of course $D[I, I]$ is the fraction of the material at I that remains at I. Then the amount of material at I at time $T+1$ is equal to $\sum_I D[I, J] \cdot \vec{v}_T[J]$, so $\vec{v}_{T+1} = M \cdot \vec{v}_T$.

Consider now a case similar to application 18 where we are considering a rectangular region, discretized into a grid of $M \times N$ interior points. Assume that the points are numbered left to right and

top to bottom, as in figure 3.3 The vector $\vec{v}$ is thus an $M \cdot N$ dimensional vector, with one dimension for each point, and D is then an $MN \times MN$ matrix. Let us say that the neighbors of a point are the four points to the left, to the right, above, and below. Assume the following values for $D[I, J]$. If $J \neq I$ then $D[I, J] = 0.1$ if J is a neighbor of I and 0 otherwise. $D[I, I]$ is 0.6 if I is an interior point with 4 neighbors; 0.7 if I is a side point with 3 neighbors; and 0.8 if I is a corner point with 2 neighbors.

A. Write a MATLAB function `DiffusionMat(M,N)` which returns the `MN` $\times$ `MN` diffusion matrix for an `M` $\times$ `N` grid of internal points.

B. Write a MATLAB function `Diffuse(Q,K)` which takes as as input argument an `M` $\times$ `N` matrix representing the grid of mass distribution at time `T` = `0` and returns the `M` $\times$ `N` grid at time `T` = `K`. Hint: You should convert Q into a vector of length `MN`, calculate the answer in terms of another vector of length `MN`, and then convert back into an `M` $\times$ `N` matrix. The MATLAB function `reshape` will be helpful.

C. Write a function `EquilibriumTime(V,EPSILON)` which computes the time `K` that it takes for all the material to "smooth out"; that is, to reach a state $\vec{V}_P$ such that the largest value in $\vec{V}_P$ minus the smallest value is less than `EPSILON`. You should use binary search. That is:

   In the first stage of the algorithm, compute in sequence the diffusion matrix D; then D^2 $D^4 = D^2 \cdot D^2$, $D^8 = D^4 \cdot D^4$ until you reach a value D^{2^k} such that $D^{2^k} \cdot \vec{v}_0$ satisfies the condition. Save all the powers of D you have computed in a 3-dimensional array.

   The exact time P is thus greater than 2^{K-1} and less than or equal to 2^K. Now, in the second stage of the algorithm, use binary search to find the exact value of P. For instance, if $K = 5$, then P is somewhere between $16 = 2^4$ and $32 = 2^5$. Try half-way between, at $(16+32)/2 = 24$. If this satisfies the condition, search between 8 and 12; if it does not, search between 12 and 16, and iterate. Note that at each stage of your search the upper bound U and the lower bound L differ by a power of 2, 2^I, and that you have already computed D^{2^I} in the first stage of the algorithm and saved it, so all you have to do now to compute the intermediate point is to multiply $D^L \cdot D^{2^I}$. Thus, you should be able to carry out the whole algorithm with at most $2\lceil \log_2 P \rceil$ matrix multiplications.

Chapter 4

Vector Spaces

This chapter is about *vector spaces*, which are certain sets of n-dimensional vectors. The material in this chapter is theoretical — concepts, definitions, and theorems. We will discuss algorithmic issues in chapter 5, and then return at length to applications in chapters 6 and 7.

There are two objectives in this chapter. The first is to discuss the structure of vector spaces; this framework will be useful in chapters 5 and 6 and necessary in chapter 7. The second is to give a characterization of the space of solutions to a system of linear equations; this follows easily from the analysis of vector spaces.

The chapter is divided into three parts, of increasing mathematical sophistication. Part I presents the material on vector spaces that we will need in the remainder of the book, while as far as possible avoiding unnecessary abstraction and mathematical difficulty. Many students will no doubt find this section quite abstract and difficult enough, but it is important that you should master the material discussed here, as it will be needed later. Part II goes over essentially the same ground, discussing some further mathematical aspects and giving proofs of theorems. Students who like abstract math will, I think, find that this material is not only interesting and mathematically very elegant, but helpful in clarifying the basic concepts and their relations. Students who do not care for abstract math may prefer to skip this. Finally, part III gives the most general definition of a vector space in the way that any self-respecting mathematician would give it. This is included so that the self-respecting mathematicians will not burn this book in the town square.

Part I

4.1 Subspaces

A *subspace* of $\mathbb{R}^n$ is a particular type of set of n-dimensional vectors. Subspaces of $\mathbb{R}^n$ are a type of *vector space*; the only kind of vector space we will consider in this book, except in part III of this chapter.

Since we are dealing extensively with sets in this chapter, we will be using the standard set operators.

$S \cup T$ is the union of S and T. $S \cap T$ is the intersection of S and T. $S \setminus T$ is the set difference S minus T; that is, the set of all elements in S but not in T. $\emptyset$ is the empty set, the set with no elements.

To begin with, we need the idea of a linear sum:

Definition 4.1. *Let $\mathcal{V}$ be a set of vectors in $\mathbb{R}^n$. A vector $\vec{u} \in \mathbb{R}^n$ is a* linear sum *over $\mathcal{V}$ if there exist $\vec{v}_1 \ldots \vec{v}_m$ in $\mathcal{V}$ and scalars $a_1 \ldots a_m$ such that $\vec{u} = a_1\vec{v}_1 + \ldots + a_m\vec{v}_m$.*

Definition 4.2. *Let $\mathcal{S}$ be a set of vectors. The* span *of $\mathcal{S}$, denoted* $\text{Span}(\mathcal{S})$ *is the set of linear sums over S.*

Example 4.1: In $\mathbb{R}^3$ let $\mathcal{V} = \{\vec{v}_1, \vec{v}_2\}$ where $\vec{v}_1 = \langle 0, 2, 0\rangle$, and $\vec{v}_2 = \langle 1, 3, -1\rangle$. Then $\text{Span}(\mathcal{V})$ is the set of all vectors $\vec{w}$ of the form $\vec{w} = a \cdot \langle 0, 2, 0\rangle + b \cdot \langle 1, 3, -1\rangle = \langle b, 2a + 3b, -b\rangle$. For instance, $\text{Span}(\mathcal{V})$ includes the vector $3\vec{v}_1 - 2\vec{v}_2 = \langle -2, 0, 2\rangle$. It does not include the vector $\langle 4, 2, -2\rangle$, because any vector $\vec{v}$ in $\text{Span}(\mathcal{V})$ satisfies $\vec{v}[3] = -\vec{v}[1]$.

Definition 4.3. *A non-empty set of n-dimensional vectors, $\mathcal{S} \subset \mathbb{R}^n$ is a* subspace *of $\mathbb{R}^n$ if $\mathcal{S} =$ $\text{Span}(\mathcal{V})$ for some set of vectors $\mathcal{V}$.*

The following theorem give a useful technique for proving that a set $\mathcal{S}$ is a subspace.

Theorem 4.1. *A non-empty set of vectors $\mathcal{S} \subset \mathbb{R}^n$ is a subspace if it is closed under the vector operations. That is, $\mathcal{S}$ satisfies the following two properties:*

- *If $\vec{u}$ and $\vec{v}$ are in $\mathcal{S}$ then $\vec{u} + \vec{v}$ are in $\mathcal{S}$.*
- *If c is a scalar and $\vec{u}$ is in $\mathcal{S}$, then $c \cdot \vec{u}$ is in $\mathcal{S}$.*

The proof is given in part II, theorem 4.12.

Example 4.2: The entire space $\mathbb{R}^n$ is a (non-strict) subspace of itself, called the "complete space".

Example 4.3: The set containing only the n-dimensional zero vector $\{\ \vec{0}\ \}$ is a subspace of $\mathbb{R}^n$ known as the "zero space".

Example 4.4: In $\mathbb{R}^2$ there are three kinds of subspaces:

1. the complete space;
2. the zero space;
3. for any line L through the origin, the set of vectors lying on L.

In case (3), the line $ax+by = 0$ is equal to $\text{Span}(\{\langle -b, a\rangle\})$. Note that a line that does not go through the origin is not a subspace. This is called an "affine space"; these will be studied in chapter 6.

Example 4.5: In $\mathbb{R}^3$ there are four kinds of subspaces: the three above, and

4. for any plane P through the origin, the vectors lying in P.

For instance, the line going equally in the x, y, z directions is equal to $\text{Span}(\{\langle 1, 1, 1\rangle\})$. The plane $x + y + z = 0$ is equal to $\text{Span}(\{\langle 1, 0, -1\rangle, \langle 0, 1, -1\rangle\})$.

Example 4.6: Consider a system of linear equations of m equations in n unknowns whose constant terms are all zero. The system can be expressed in the form $M\vec{x} = \vec{0}$; this is known as a *homogeneous* system of equations. Let $\mathcal{S}$ be the set of all solutions to this system. We can use theorem 4.1 to show that $\mathcal{S}$ is a subspace of $\mathbb{R}^n$:

- If $\vec{u}$ and $\vec{v}$ are in $\mathcal{S}$, then $M\vec{u} = \vec{0}$ and $M\vec{v} = 0$. Then $M(\vec{u} + \vec{v}) = M\vec{u} + M\vec{v} = \vec{0} + \vec{0} = \vec{0}$ so $\vec{u} + \vec{v}$ is in $\mathcal{S}$.
- If $\vec{u}$ is in $\mathcal{S}$ and c is a scalar then $M(c\vec{v}) = c \cdot M\vec{v} = c \cdot \vec{0} = \vec{0}$, so $c\vec{u}$ is in $\mathcal{S}$.

Example 4.7: Suppose that a retail store keeps a database with a record for each item. The record for item I is a three-dimensional vector, consisting of the price paid for I, the price at which I was sold, and the net profit or loss on I. Then a vector $\vec{v}$ is a legitimate entry just if it satisfies the equation $\vec{v}[3] = \vec{v}[2] - \vec{v}[1]$ (profit is selling price minus buying price). Therefore, the set of legitimate entries is a subspace of $\mathbb{R}^3$.

Of course, it is not quite accurate to say that any vector that satisfies the condition is an actually possible entry. Consider the vectors $\langle -2, -9, -7\rangle$, $\langle 2\pi, 9\pi, 7\pi\rangle$, and $\langle 2 \cdot 10^{30}, 9 \cdot 10^{30}, 7 \cdot 10^{30}\rangle$. Any of these is likely to raise suspicions in an auditor, because it is not usual to buy or sell an item for a negative value, for an irrational value, or for more money than exists in the world. It would be more accurate to say that the set of legitimate values is a subset of the subspace of values satisfying $\vec{v}[3] = \vec{v}[2] - \vec{v}[1]$. However, we will ignore that inconvenient reality.

Example 4.8: Consider an alternative version of the previous example, where an international business records price, cost, and profit in a number of different currencies; and let us suppose, unrealistically, that the exchange rates are constant over time. Specifically, the database records the three amounts in dollars, Euros, and yen, and we will suppose that 1 dollar = 0.8 euro = 90 yen. Then a valid entry is a 9-tuple satisfying the equations:

$$\begin{aligned}
\vec{v}[3] &= \vec{v}[2] - \vec{v}[1] \\
\vec{v}[4] &= 0.8 \cdot \vec{v}[1] \\
\vec{v}[5] &= 0.8 \cdot \vec{v}[2] \\
\vec{v}[6] &= 0.8 \cdot \vec{v}[3] \\
\vec{v}[7] &= 90 \cdot \vec{v}[1] \\
\vec{v}[8] &= 90 \cdot \vec{v}[2] \\
\vec{v}[9] &= 90 \cdot \vec{v}[3]
\end{aligned}$$

4.2 Coordinates, bases, linear independence

Suppose that we have a subspace $\mathcal{V}$ of $\mathbb{R}^n$. We want to construct a *coordinate system* for $\mathcal{V}$; that is, a notation that represents all and only vectors in $\mathcal{V}$. That way, we can be sure that all of our records are valid vectors in $\mathcal{V}$, since the notation can *only* express vectors in $\mathcal{V}$.

The standard way to construct a coordinate system is by using a *basis* for $\mathcal{V}$. A basis for $\mathcal{V}$ is a finite tuple $\mathcal{B} = \langle \vec{b}_1 \ldots \vec{b}_m \rangle$, satisfying two conditions that we will state below. If $\vec{u}$ is a vector in $\mathcal{V}$, then the *coordinates of $\vec{u}$ in basis $\mathcal{B}$*, denoted "Coords($\vec{u}, \mathcal{B}$)", is the sequence $\langle a_1 \ldots a_m \rangle$ such that $\vec{u} = a_1\vec{b}_1 + \ldots + a_m\vec{b}_m$.

Now, in order for this to be a legitimate coordinate system, it must satisfy two conditions:

- Any tuple of coordinates must represent a vector in $\mathcal{V}$, and and every vector in $\mathcal{V}$ must be representable as a tuple of coordinates over $\mathcal{B}$ — that is, as a linear sum over $\mathcal{B}$. Therefore, we must choose $\mathcal{B}$ so that $\text{Span}(\mathcal{B}) = \mathcal{V}$.
- A single vector $\vec{u}$ has only one tuple of coordinates in $\mathcal{B}$; that is, any two different sets of coordinates give different vectors. This is guaranteed by requiring that $\mathcal{B}$ is *linearly independent* (defined below).

Definition 4.4. *A set of vectors $\mathcal{V}$ is* linearly dependent *if one of the vectors in $\mathcal{V}$ is a linear sum of the rest. That is, for some $\vec{v} \in \mathcal{V}$, $\vec{v} \in \text{Span}(\mathcal{V} \setminus \{\vec{v}\})$. $\mathcal{V}$ is* linearly independent *if it is not linearly dependent.*

We can now define a basis:

Definition 4.5. *Let $\mathcal{V}$ be a subspace of $\mathbb{R}^n$. A finite subset $\mathcal{B} \subset \mathcal{V}$ is a* basis *for $\mathcal{V}$ if*

a. $\text{Span}(\mathcal{B}) = \mathcal{V}$.

b. $\mathcal{B}$ is linearly independent.

The following theorem states that a basis $\mathcal{B}$ for a subspace $\mathcal{S}$ defines a coordinate system with the desired properties:

Theorem 4.2. *Let $\mathcal{B} = \langle \vec{b}_1 \dots \vec{b}_m \rangle$ be a basis for vector space $\mathcal{S}$ and let $\vec{v}$ be a vector in $\mathcal{S}$. Then:*

a. For any vector $\vec{v} \in \mathcal{S}$, there exists a unique m-tuple of coordinates $\langle a_1 \dots a_m \rangle = \text{Coords}(\vec{v}, \mathcal{B})$ such that $\vec{v} = a_1\vec{b}_1 + \dots + a_m\vec{b}_m$.

b. For any m-tuple of coordinates $\langle a_1 \dots a_m \rangle$ the linear sum $\vec{v} = a_1\vec{b}_1 + \dots + a_m\vec{b}_m$ is in $\mathcal{S}$.

The proof of (a) is given in part II, theorem 4.16. Part (b) follows directly from the definitions.

In order to be able to include the zero space in our theorems about subspaces, it is convenient to adopt the following conventions:

- The zero space is considered to be the span of the empty set: $\{\vec{0}\} = \text{Span}(\emptyset)$. You get the zero vector for free, so to speak.
- The empty set is considered to be linearly independent.
- The set containing just the zero vector $\{\vec{0}\}$ is considered to be linearly dependent.

4.2.1 Examples of bases and coordinates

Any vector space, other than the zero space, has many different bases. Here are some examples of bases for the vector spaces discussed above.

A basis for all of $\mathbb{R}^n$ is the set $\langle e^1, e^2 \dots e^n \rangle$. (Recall that e^i is the vector whose ith component is 1 and other components are 0.)

A basis for the line $ax + by = 0$ is the singleton set $\{\langle b, -a \rangle\}$. In fact, if $\vec{v}$ is any non-zero vector in the line, then $\{\vec{v}\}$ is a basis for the line.

A basis for the plane $x + y + z = 0$ is the pair of vectors $\{\langle 1, -1, 0 \rangle, \langle 1, 0, -1 \rangle\}$. Another basis is the pair $\{\langle 1, 1, -2 \rangle, \langle -2, 1, 1 \rangle\}$. In fact, any two non-collinear vectors in this plane form a basis.

A basis for the space described in example 4.7 is the pair $\{\langle 1, 0, -1 \rangle, \langle 0, 1, 1 \rangle\}$. Another basis is the pair $\{\langle 0, 1, 1 \rangle, \langle 1, 1, 0 \rangle\}$.

We leave it as an exercise to find a basis for the space described in example 4.8.

Example 4.9: Let us go back to the plane $x + y + z = 0$. We identified above two bases for this subspace:

- $\mathcal{B} = \{\vec{b}_1, \vec{b}_2\}$ where $\vec{b}_1 = \langle 1, 0, -1\rangle$ and $\vec{b}_2 = \langle 0, 1, -1\rangle$.
- $\mathcal{C} = \{\vec{c}_1, \vec{c}_2\}$ where $\vec{c}_1 = \langle 1, 1, -2\rangle$ and $\vec{c}_2 = \langle -2, 1, 1\rangle$.

We will use each of these as coordinate systems. Let us take two particular vectors in the plane: $\vec{u} = \langle -5, 7, -2\rangle$ and $\vec{v} = \langle 1, 8, -9\rangle$. Measuring these in coordinate system $\mathcal{B}$, these have the following coordinates:

- $\text{Coords}(\vec{u}, \mathcal{B}) = \langle -5, 7\rangle$ because $5 \cdot \vec{b}_1 + 7 \cdot \vec{b}_2 = \vec{u}$.
- $\text{Coords}(\vec{v}, \mathcal{B}) = \langle 1, 8\rangle$ because $1 \cdot \vec{b}_1 + 8 \cdot \vec{b}_2 = \vec{v}$.

On the other hand, measuring them in coordinate system $\mathcal{C}$, they have the following coordinates:

- $\text{Coords}(\vec{u}, \mathcal{C}) = \langle 3, 4\rangle$ because $3 \cdot \vec{c}_1 + 4 \cdot \vec{c}_2 = \vec{u}$.
- $\text{Coords}(\vec{v}, \mathcal{C}) = \langle 17/3, 7/3\rangle$ because $17/3 \cdot \vec{c}_1 + 7/3 \cdot \vec{c}_2 = \vec{v}$.

It is easy to *check* that these are the correct coordinates by doing the above sums; we will discuss in chapter 7 how you can *find* the coordinates of a vector relative to a given basis.

4.2.2 Properties of bases and coordinates

As we said, any subspace has many different bases. But, as the above examples suggest, the different bases of a subspace have a very important property in common; they all have the same number of elements.

Theorem 4.3. *Let $\mathcal{V}$ be a subspace of $\mathbb{R}^n$. Then any two bases for $\mathcal{V}$ have the same number of elements. This is known as the* dimension *of $\mathcal{V}$, denoted* $\text{Dim}(\mathcal{V})$. *By convention, the dimension of the zero space is 0.*

The proof is given in part II, corollary 4.18.

Now, suppose that $\mathcal{V}$ is an m-dimensional vector space, and $\mathcal{B}$ is a basis for $\mathcal{V}$. Then for any vector $\vec{u}$ in $\mathcal{V}$, the coordinates for $\vec{u}$ in terms of $\mathcal{B}$, $\text{Coords}(\vec{u}, \mathcal{B}) = \langle a_1 \dots a_m\rangle$, is itself an m-dimensional vector. The great thing about this coordinate notation is that you can carry out vector operations on the *actual* vectors by applying the operators to their *coordinates* in any basis.

Theorem 4.4. *Let $\mathcal{V}$ be a subspace of $\mathbb{R}^n$ and let $\mathcal{B}$ be a basis for $\mathcal{V}$. Then*

- *For any $\vec{u}, \vec{w} \in \mathcal{V}$,* $\text{Coords}(\vec{u} + \vec{w}, \mathcal{B}) = \text{Coords}(\vec{u}, \mathcal{B}) + \text{Coords}(\vec{w}, \mathcal{B})$
- *For any $\vec{u} \in \mathcal{V}$ and scalar a,* $\text{Coords}(a \cdot \vec{u}, \mathcal{B}) = a \cdot \text{Coords}(\vec{u}, \mathcal{B})$.
- *The coordinates of a linear sum is equal to the linear sum of the coordinates. That is*

$$\text{Coords}(a_1 \cdot \vec{v}_1 + \ldots + a_n \cdot \vec{v}_n, \mathcal{B}) = a_1 \cdot \text{Coords}(\vec{v}_1, \mathcal{B}) + \ldots + a_n \cdot \text{Coords}(\vec{v}_n, \mathcal{B})$$

The proof is left as an exercise (Problem 4.1).

For instance, let us go back to example 4.7. Suppose that we have decided to use the coordinate system $\mathcal{C}$ and we have recorded that $\text{Coords}(\vec{u}, \mathcal{C}) = \langle 3, 4\rangle$ and $\text{Coords}(\vec{v}, \mathcal{C}) = \langle 17/3, 7/3\rangle$. We want to now compute $\text{Coords}(6\vec{v} - 2\vec{u}, \mathcal{C})$. One way would be to translate $\vec{u}$ and $\vec{v}$ back into their native form, do the computation, and then translate the result back into coordinates relative to $\mathcal{C}$. But theorem 4.4 gives us a much simpler solution:

$$\text{Coords}(6\vec{v} - 2\vec{u}, \mathcal{C}) = 6\,\text{Coords}(\vec{v}, \mathcal{C}) - 2\,\text{Coords}(\vec{u}, \mathcal{C}) = \langle 28, 6\rangle$$

4.3 Orthogonal and orthonormal basis

An *orthogonal basis* is one where every pair of elements is orthogonal. For instance, the subspace $x + y + z = 0$ has the orthogonal basis $\mathcal{O} = \{\langle 1, -1, 0\rangle, \langle 1, 1, -2\rangle\}$.

An *orthonormal basis*[1] is an orthogonal basis in which every element has length 1. If $\mathcal{B}$ is an orthogonal basis for space $\mathcal{S}$, then you can get an orthonormal basis by dividing each element in $\mathcal{B}$ by its length. basis by dividing each basis vector by its length. For instance, in the orthogonal basis $\mathcal{O}$ above for the space $x + y + z = 0$, the first vector has length $\sqrt{2}$ and the second has length $\sqrt{6}$. Therefore, this turns into the orthonormal basis $\mathcal{N} = \langle 1/\sqrt{2},\ -1/\sqrt{2},\ 0\rangle, \langle 1/\sqrt{6},\ 1/\sqrt{6},\ -2/\sqrt{6}\rangle$.

The obvious drawback of using orthonormal bases is that you get involved with irrational numbers. But the advantage is that, if vectors in $\mathcal{V}$ are recorded in terms of their coordinates in an orthonormal basis, then lengths and dot products can also be computed without translating back to the standard coordinates.

Theorem 4.5. *Let $\mathcal{V}$ be a vector space and let $\mathcal{B}$ be an orthonormal basis for V. Then:*

- *For any $\vec{u}, \vec{w} \in \mathcal{V}$, $\vec{u} \bullet \vec{w} = \text{Coords}(\vec{u}, \mathcal{B}) \bullet \text{Coords}(\vec{w}, \mathcal{B})$.*
- *For any $\vec{u} \in \mathcal{V}$, $|\vec{u}| = |\,\text{Coords}(\vec{u}, \mathcal{B})|$.*

The proof is in part II, theorem 4.28.

We again illustrate using the subspace $x+y+z = 0$. As above, let $\vec{u} = \langle -5, 7, -2\rangle$ and $\vec{v} = \langle 1, 8, -9\rangle$. Then

$$\begin{array}{l}\text{Coords}(\vec{u}, \mathcal{O}) = \langle -6, 1\rangle \text{ and } \text{Coords}(\vec{v}, \mathcal{O}) = \langle -7/2, 9/2\rangle,\\ \text{so } \text{Coords}(\vec{u}, \mathcal{N}) = \langle -6\sqrt{2}, \sqrt{6}\rangle = \langle 8.4852, 2.4495\rangle \text{ and}\\ \text{Coords}(\vec{v}, \mathcal{N}) = \langle -7\sqrt{2}/2,\ 9\sqrt{6}/2\rangle = \langle 4.9497, 11.0227\rangle.\end{array}$$

We leave it as an exercise (exercise 4.3) to check that, as theorem 4.5 claims,

$$\begin{array}{l}|\vec{u}| = |\,\text{Coords}(\vec{u}, \mathcal{N})| = \sqrt{74};\\ |\vec{v}| = |\,\text{Coords}(\vec{v}, \mathcal{N})| = \sqrt{146}; \text{ and}\\ \vec{u} \bullet \vec{v} = \text{Coords}(\vec{u}, \mathcal{N}) \bullet \text{Coords}(\vec{v}, \mathcal{N}) = 69.\end{array}$$

An orthonormal basis also have the following important and elegant property:

Theorem 4.6. *Let $\mathcal{B} = \{\vec{b}_1 \ldots \vec{b}_q\}$ be an orthonormal basis for vector space $\mathcal{V}$. If $\vec{v}$ is a vector in $\mathcal{V}$, then the ith coordinate of $\vec{v}$ with respect to $\mathcal{B}$,* $\text{Coords}(\vec{v}, \mathcal{B})[i] = \vec{v} \bullet \vec{b}_i$.

The proof is in part II, theorem 4.29.

A matrix M is orthonormal if its columns are orthonormal. Square orthonormal matrices have the following properties, which will be important in chapter 7:

Theorem 4.7. *If M is an $n \times n$ orthonormal matrix, then M^T is also orthonormal and $M \cdot M^T = M^T \cdot M = I_n$.*

We leave the proof of this as an exercise (Problem 4.2).

[1] Unhelpfully, in the mathematical literature, the term "orthogonal basis" is often used to mean "orthonormal basis".

4.4 Operations on vector spaces

There are two important ways in which you can combine two subspaces $\mathcal{U}$ and $\mathcal{V}$ of $\mathbb{R}^n$. First, you can take their intersection $\mathcal{U} \cap \mathcal{V}$. Second, you can take their *direct sum,* denoted $\mathcal{U} \oplus \mathcal{V}$, which is defined as $\mathcal{U} \oplus \mathcal{V} = \text{Span}(\mathcal{U} \cup \mathcal{V})$. Both $\mathcal{U} \cap \mathcal{V}$ and $\mathcal{U} \oplus \mathcal{V}$ are themselves vector spaces.

In two dimensions, the direct sum of two distinct lines is the entire space; their intersection is the zero space. In three dimensional space, if $\mathcal{U}$ and $\mathcal{V}$ are different lines, then $\mathcal{U} \oplus \mathcal{V}$ is the plane containing them. If $\mathcal{U}$ is a plane and $\mathcal{V}$ is a line outside $\mathcal{U}$, then $\mathcal{U} \oplus \mathcal{V}$ is the entire space.

Theorem 4.8 states three important properties of these operations.

Theorem 4.8. *Let $\mathcal{U}$ and $\mathcal{V}$ be subspaces of $\mathbb{R}^n$.*

a. *For any vector $\vec{w}$ in $\mathcal{U} \oplus \mathcal{V}$, there exists $\vec{u} \in \mathcal{U}$ and $\vec{v} \in \mathcal{V}$ such that $\vec{w} = \vec{u} + \vec{v}$. If $\mathcal{U} \cap \mathcal{V} = \{\vec{0}\}$, then there is only one possible choice of $\vec{u}$ and $\vec{v}$.*

b. *If $\mathcal{U} \cap \mathcal{V} = \{\vec{0}\}$ then the union of a basis for $\mathcal{U}$ with a basis for $\mathcal{V}$ is a basis for $\mathcal{U} \oplus \mathcal{V}$.*

c. $\text{Dim}(\mathcal{U} \oplus \mathcal{V}) = \text{Dim}(\mathcal{U}) + \text{Dim}(\mathcal{V}) - \text{Dim}(\mathcal{U} \cap \mathcal{V})$

The proof of (c) is given in part II, theorem 4.26. The proofs of (a) and (b) are left as exercises (problem 4.3).

Two vector spaces $\mathcal{U}$ and $\mathcal{V}$ are *complements* if $\mathcal{U} \cap \mathcal{V} = \{\vec{0}\}$ and $\mathcal{U} \oplus \mathcal{V} = \mathbb{R}^n$. If $\mathcal{U}$ and $\mathcal{V}$ are complements, then any vector in $\mathbb{R}^n$ can be written in exactly one way as the sum of a vector in $\mathcal{U}$ plus a vector in $\mathcal{V}$. $\mathcal{U}$ and $\mathcal{V}$ are *orthogonal complements* if they are complements, and any vectors $\vec{u} \in \mathcal{U}$ and $\vec{v} \in \mathcal{V}$ are orthogonal. In fact, the orthogonal complement of $\mathcal{U}$ is just the set of all vectors $\vec{v}$ such that $\vec{c}$ is orthogonal to every vector in $\mathcal{U}$.

Theorem 4.9. *Any subspace of $\mathbb{R}^n$ has an orthogonal basis and an orthogonal complement.*

The proof is in part II, theorem 4.31.

If $\mathcal{U}$ and $\mathcal{V}$ are complements, then $\mathcal{U} \oplus \mathcal{V} = \mathbb{R}^n$ so $\text{Dim}(\mathcal{U} \oplus \mathcal{V}) = n$, and $\mathcal{U} \cap \mathcal{V} = \{\vec{0}\}$ so $\text{Dim}(\mathcal{U} \cap \mathcal{V}) = 0$. So using the formula above we have $\text{Dim}(\mathcal{U}) + \text{Dim}(\mathcal{V}) = \text{Dim}(\mathcal{U} \oplus \mathcal{V}) + \text{Dim}(\mathcal{U} \cap \mathcal{V}) = n$. So, for example, in two dimensions, any two distinct lines through the origin are complements. In three dimensions a plane P through the origin and any line L through the origin not lying in P are complements.

4.5 Null space, image space, and rank

We can now use the theory of vector spaces that we have developed above to partially characterize what a linear transformation does.

Suppose that Γ is a linear transformation from $\mathbb{R}^n$ to $\mathbb{R}^m$. Then the *image* of Γ, $\text{Image}(\Gamma) = \Gamma(\mathbb{R}^n)$. This is a subspace of $\mathbb{R}^m$. The *null space* (also called the *kernel*) of Γ is the set of vectors in $\mathbb{R}^n$ that Γ maps to $\vec{0}$.

$$\text{Null}(\Gamma) = \{\vec{v} \in \mathbb{R}^n \mid \Gamma(\vec{v}) = \vec{0}\}$$

Now, let $\mathcal{V}$ be any subspace of $\mathbb{R}^n$ that is complementary to $\text{Null}(\Gamma)$. Since $\text{Null}(\Gamma)$ and $\mathcal{V}$ are complementary, any vector $\vec{p} \in \mathbb{R}^n$ is equal to $\vec{u} + \vec{v}$ where $\vec{u} \in \text{Null}(\Gamma)$ and $\vec{v} \in \mathcal{V}$. Then $\Gamma(\vec{p}) =$

$\Gamma(\vec{u}+\vec{v}) = \Gamma(\vec{u}) + \Gamma(\vec{v}) = \Gamma(\vec{v})$. Thus any vector in Image(Γ) is in $\Gamma(\mathcal{V})$. In fact one can show that Γ is a *bijection* between $\mathcal{V}$ and Image(Γ); that is, for every vector $\vec{w} \in$ Image(Γ) there exists exactly one vector $\vec{v} \in V$ such that $\vec{w} = \Gamma(\vec{v})$.

So one can think about what Γ does in this way. You identify Null(Γ), the set of vectors that Γ sends to $\vec{0}$. You choose some vector space $\mathcal{V}$ that is complementary to Null(Γ). (Note that there are many ways to choose $\mathcal{V}$, though there is no choice about Null(Γ). If you like, you *may* choose $\mathcal{V}$ to be the orthogonal complement to Null(Γ) and sometimes that is the best choice, but not always.) You can then divide any vector $\vec{p} \in \mathbb{R}^n$ into a component $\vec{u} \in$ Null(Γ) and a component $\vec{v}$ in $\mathcal{V}$, such that $\vec{p} = \vec{v} + \vec{u}$. When Γ is applied to $\vec{p}$, it simply zeros out the $\vec{u}$ component, and sets $\Gamma(\vec{p}) = \Gamma(\vec{v})$.

How do we describe what Γ does to vectors in $\mathcal{V}$? The easiest way is to choose a basis for $\mathcal{V}$. If $\vec{b}_1 \ldots \vec{b}_r$ is a basis for $\mathcal{V}$, then $\Gamma(\vec{b}_1) \ldots \Gamma(\vec{b}_r)$ is a basis for Image(Γ). Moreover, if $\vec{v}$ is any vector in $\mathcal{V}$, then the coordinates of $\Gamma(\vec{v})$ with respect to the basis $\{\Gamma(\vec{b}_1) \ldots \Gamma(\vec{b}_r)\}$ are the same as the coordinates of $\vec{v}$ with respect to the basis $\{\vec{b}_1 \ldots \vec{b}_r\}$.

Note that we now have *two* important uses for bases:

- To serve as the basis for a coordinate system.
- To use in characterizing linear transformations.

The number r above is the dimension both of $\mathcal{V}$ and of Image(Γ). This is known as the *rank* of Γ: Rank(Γ) = Dim(Image(Γ)).

One further point. Since $\mathcal{V}$ and Image(Γ) have bases of the same size, we have Dim($\mathcal{V}$) = Dim(Image(Γ)) = Rank(Γ). But since $\mathcal{V}$ and Null(Γ) are complementary subspaces of $\mathbb{R}^n$, we have Dim($\mathcal{V}$)+Dim(Null(Γ)) = n, so Dim(Null(Γ)) = n − Rank(Γ).

These functions apply to matrices in the same way; that is, if M is the matrix corresponding to transformation Γ, then Image(M) = Image(Γ), Null(M) = Null(Γ), Rank(M) = Rank(Γ). The following theorem applies to these properties of matrices:

Theorem 4.10. *For any matrix M:*

- Image(M) *is the space spanned by the columns of M. Therefore* Rank(M) = Dim(Image(M)) *is the dimension of the space spanned by the columns of M.*
- Rank(M) *is also the dimension of the space spanned by the* rows *of M. Therefore* Rank(M) = Rank(M^T).

The proof is in part II, theorem 4.37 and corollary 4.52.

Example 4.10 Let M be the matrix:

$$M = \begin{bmatrix} 1 & 2 & -1 \\ 3 & 6 & -3 \end{bmatrix}$$

Then Null(M) is the set of vectors $\langle x, y, z\rangle$ such that $x + 2y - z = 0$ and $3x + 6y - 3z = 0$. Since any vector that satisfies the first also satisfies the second, this is just the plane $x + 2y - z = 0$. We can choose for $\mathcal{V}$ any complement of Null(M). Since Null(M) is 2 dimensional, $\mathcal{V}$ must be 1 dimensional, so we may choose as a basis any vector $\vec{b}$ that does not lie in the plane Null(M). Let us choose $\vec{b} = \langle 1, 0, 0\rangle$, the unit x-vector, and basis $\mathcal{B} = \{\vec{b}\}$, so $\mathcal{V} =$ Span($\mathcal{B}$) $= \{t \cdot \langle 1, 0, 0\rangle\}$, the set of vectors on the x-axis.

Now $M \cdot \vec{b} = \langle 1, 3\rangle$. The image of M is given by

$$\text{Image}(M) = \{M \cdot \vec{v} \mid \vec{v} \in \mathcal{V}\} = \{M \cdot t \cdot \langle 1, 0, 0\rangle\} = \text{Span}(M \cdot \vec{b}) = \{t \cdot \langle 1, 3\rangle\}$$

This is the line in the plane with slope 3.

Consider a vector in $\mathbb{R}^3$, say $\vec{w} = \langle 9, 2, 6\rangle$. We can then find vectors $\vec{u} \in \text{Null}(M)$ and $\vec{v} \in \mathcal{V}$ such that $\vec{w} = \vec{u} + \vec{v}$. In this case $\vec{u} = \langle 2, 2, 6\rangle$ and $\vec{v} = \langle 7, 0, 0\rangle$. Then $M \cdot \vec{w} = M \cdot \vec{v} = \langle 7, 21\rangle$. Note that $\text{Coords}(\vec{v}, \mathcal{B}) = \text{Coords}(M \cdot \vec{v}, \{M \cdot \vec{b}\}) = \langle 7\rangle$.

Example 4.11 Let M be the matrix

$$M = \begin{bmatrix} 1 & 2 & -1 \\ -1 & 0 & 1 \\ -1 & 2 & 1 \end{bmatrix}$$

Then $\text{Null}(M)$ is the one-dimensional line $\{t \cdot \vec{n}\}$. where $\vec{n}$ is the vector $\langle 1, 0, 1\rangle$. The complementary space $\mathcal{V}$ is thus a two-dimensional plane. As a basis $\mathcal{B}$ for the complementary space, we may take any two non-collinear vectors that do not lie in $\text{Null}(M)$, We will take $\vec{b}_1 = \langle 0, 1, 1\rangle$ and $\vec{b}_2 = \langle 1, 1, 0\rangle$. Then

$$\mathcal{V} = \text{Span}(\mathcal{B}) = \{a_1 \cdot \vec{b}_1 + a_2 \cdot \vec{b}_2\} = \{\langle a_1, a1 + a_2, a_2 \mid a_1, a_2 \in \mathbb{R}\}$$

You can check that these are indeed the null space and a complementary space by checking that

a. $M \cdot \vec{n} = \vec{0}$.

b. $M \cdot \vec{b}_1 \neq \vec{0}$, and $M \cdot \vec{b}_2 \neq \vec{0}$. So these are not in the null space.

c. $\vec{b}_1$ and $\vec{b}_2$ are linearly independent.

It follows from (a) that $\text{Span}(\{\vec{n}\})$ is in the null space, and from (b) and (c) it follows that $\text{Span}(\mathcal{B})$ is in a complementary space. But since we have now used up all three dimensions, it follows that $\text{Span}(\{\vec{n}\})$ is the complete null space and that $\text{Span}(\mathcal{B})$ is a complete complement.

Now $\{M \cdot \vec{b}_1, M \cdot \vec{b}_2\} = \{\langle 1, 1, 3\rangle, \langle 3, -1, 1\rangle\}$.
So $\text{Image}(M) = \text{Span}(\{M \cdot \vec{b}_1, M \cdot \vec{b}_2\}) = \{a_1 \cdot \langle 1, 1, 3\rangle + a_2 \cdot \langle 3, -1, 1\rangle\}$,
the plane spanned by $\langle 1, 1, 3\rangle$ and $\langle 3, -1, 1\rangle$.

Consider a vector in $\mathbb{R}^3$, say $\vec{w} = \langle 5, 3, 4\rangle$. We can then find vectors $\vec{u} \in \text{Null}(M)$ and $\vec{v} \in \mathcal{V}$ such that $\vec{w} = \vec{u} + \vec{v}$. In this case $\vec{u} = \langle 3, 0, 3\rangle$ and $\vec{v} = \langle 2, 3, 1\rangle$. Then $M \cdot \vec{w} = M \cdot \vec{v} = \langle 7, -1, 5\rangle$. Note that $\text{Coords}(\vec{v}, \mathcal{B}) = \text{Coords}(M\vec{v}, \{M \cdot \vec{b}_1, M \cdot \vec{b}_2\}) = \langle 1, 2\rangle$.

4.6 Systems of linear equations

We now apply all this theory to systems of linear equations. Let M be an $m \times n$ matrix.

First we note that the null space of M is the set of vectors $\vec{x}$ such that $M\vec{x} = \vec{0}$; that is, it is the set of solutions to the system $M\vec{x} = \vec{0}$ of m equations in n unknowns.

Second, let us think about the system of equations $M\vec{x} = \vec{c}$. This has a solution if $\vec{c}$ is in $\text{Image}(M)$. Therefore, if $\text{Image}(M) = \mathbb{R}^m$ — that is, $\text{Rank}(M) = m$ — then every vector $\vec{c}$ in $\mathbb{R}^m$ is in $\text{Image}(M)$, so the system of equations has a solution for every $\vec{c}$. If $\text{Rank}(M) < m$, then $\text{Image}(M)$ is a proper subset of $\mathbb{R}^m$, so most vectors $\vec{c}$ that are in $\mathbb{R}^m$ are not in $\text{Image}(M)$ and for those, the system $M\vec{x} = \vec{c}$ has no solution.

On the other hand, suppose $\vec{q}$ satisfies $M\vec{x} = \vec{c}$ and suppose that some non-zero vector $\vec{u}$ is in $\text{Null}(M)$. Then $M(\vec{q} + \vec{u}) = M\vec{q} = \vec{c}$, so $\vec{q} + \vec{u}$ also satisfies the system $M\vec{x} = \vec{c}$. The converse is also true; if $\vec{q}$ and $\vec{p}$ are two solutions of the system $M\vec{x} = \vec{c}$ then

$$M(\vec{p} - \vec{q}) = M\vec{p} - M\vec{q} = \vec{c} - \vec{c} = \vec{0}$$

So $\vec{p} - \vec{q}$ is in Null(M).

The set of all solutions to the system of equations $M\vec{x} = \vec{c}$ therefore has the form $\{\vec{b}+\vec{u} | \vec{u} \in \text{Null}(M)\}$. In general, a set of this form $\{\vec{p}+\vec{u} | \vec{u} \in \mathcal{U}$, where $\mathcal{U}$ is a subspace of $\mathbb{R}^n$ is called an *affine* space.

Therefore there are two critical features of a matrix M that determine the characteristics of the solutions to the system of equations $M\vec{x} = \vec{c}$. Each feature has two possibilities, giving four combinations.

Feature A: The image.

Case 1: Image(M) is all of $\mathbb{R}^m$. This holds if Rank(M) $= m$. In this case, the system $M\vec{x} = \vec{c}$ has at least one solution for every $\vec{c}$.

Case 2: Image(M) is a proper subset of $\mathbb{R}^m$. This holds if Rank(M) $< m$. In this case, the system $M\vec{x} = \vec{c}$ has no solution for any $\vec{c}$ which is in $\mathbb{R}^m$ but not in Image(M).

Feature B: The null space.

Case A: Null(M) is just the zero space. This holds if Rank(M) $= n$. In this case, the system $M\vec{x} = \vec{c}$ has at most one solution for any $\vec{c}$.

Case B: Null(M) contains non-zero vectors. This holds if Rank(M) $< n$. In this case, for any value $\vec{c}$, if the system $M\vec{x} = \vec{c}$ has any solutions, then it has infinitely many solutions.

Let us now consider systems of equations $M\vec{x} = \vec{c}$, of m equations in n unknowns (that is, M is an $m \times n$ matrix). Keeping M fixed, but allowing $\vec{c}$ to vary, there are four categories, corresponding to the combinations of the cases above.

Category I: Image(M) $= \mathbb{R}^m$. Null(M) $= \{\vec{0}\}$. $n = m =$ Rank(M). For any $\vec{c}$ there exists exactly one solution.

Category II: Image(M) $= \mathbb{R}^m$. Null(M) $\neq \{\vec{0}\}$. Dim(Null(M)) $= n - m > 0$. $m =$ Rank(M) $< n$. For any $\vec{c}$ there exist infinitely many solutions.

Category III: Image(M) $\neq \mathbb{R}^m$. Null(M) $= \{\vec{0}\}$. $n =$ Rank(M) $< m$. Dim(Image(M)) $=$ Rank(M) $< m$, so Image(M) does not include all of $\mathbb{R}^m$. Null(M) $= \{\vec{0}\}$. For $\vec{c} \in$ Image(M) there exists a unique solution; for $\vec{c} \notin$ Image(M), there does not exist any solution.

Category IV: Image(M) $\neq \mathbb{R}^m$. Null(M) $\neq \{\vec{0}\}$. Rank(M) $< m$, Rank(M) $< n$. Dim(Image(M)) $=$ Rank(M) $< m$, so Image(M) does not include all of $\mathbb{R}^m$. Dim(Null(M)) $= n -$ Rank(M) > 0. For $\vec{c} \in$ Image(M) there exists infinitely many solutions; for $\vec{c} \notin$ Image(M), there does not exist any solution.

4.7 Inverses

Let M be a category I matrix; that is, an $n \times n$ matrix of rank n. Then the linear transformation $\Gamma(\vec{v}) = M \cdot \vec{v}$ is a bijection from $\mathbb{R}^n$ to itself; that is, for every $\vec{w} \in \mathbb{R}^n$ there exists exactly one $\vec{v} \in \mathbb{R}^n$ such that $\Gamma(\vec{v}) = \vec{w}$. Therefore, we can define an inverse Γ^{-1} where $\Gamma^{-1}(\vec{w})$ is the unique $\vec{v}$ such that $\Gamma(\vec{v}) = \vec{w}$. In other words, $\Gamma^{-1}(\Gamma(\vec{v})) = \vec{v} = \Gamma(\Gamma^{-1}(\vec{v}))$.

It is easy to show (theorem 4.43 below) that in fact Γ^{-1} must be a linear transformation. Therefore there exists an $n \times n$ matrix corresponding to Γ. This is called the *inverse* of M and is denoted M^{-1}. Since $\Gamma \circ \Gamma^{-1}$ and $\Gamma^{-1} \circ \Gamma$ are both the identity mapping from $\mathbb{R}^n$ to itself, it follows that $M \cdot M^{-1} = M^{-1} \cdot M = I^n$, the $n \times n$ identity matrix.

Now, suppose you have a system of linear equations $M \cdot \vec{x} = \vec{c}$. Multiplying both sides by M^{-1} gives you $M^{-1}M\vec{x} = \vec{x} = M^{-1}\vec{c}$, so you have solved the system! In practice, as we will discuss in chapter 5, this is not actually an effective way to solve one particular system of linear equations. However, if you will often need to solve systems of the form $M\vec{x} = \vec{c}$, with the same value of M but different values of $\vec{c}$, then this may be a good approach; compute M^{-1} once and for all and then just do the matrix multiplication $M^{-1}\vec{c}$ for each different value of $\vec{c}$.

4.8 Null space and Rank in MATLAB

The MATLAB function `rank(A)`, returns the rank of matrix A. The function `null(A)` returns a matrix whose columns are an orthonormal basis for the null space of matrix A. (These use a tolerance for closeness of the relevant quantities to zero, which can be set using an optional parameter.)

Example:

```
>> a=[1,2,3,4 ; 1,1,1,1 ; 2,3,4,5; 0,1,2,3]
a =
     1     2     3     4
     1     1     1     1
     2     3     4     5
     0     1     2     3

%

>> rank(a)
ans =
     2

>> q=null(a)
q  =
    0.4689   -0.2831
   -0.4142    0.7270
   -0.5783   -0.6046
    0.5236    0.1607

>> a*q
ans =
   1.0e-14 *
         0    0.0888
   -0.0111    0.0444
         0    0.1554
         0    0.0389

>> q'*q
ans =
    1.0000   -0.0000
   -0.0000    1.0000
```

Part II: Proofs and other abstract mathematics : Optional

In this part, we give proofs for the theorems (except those whose proofs we leave as an exercise.) We also introduce some more abstract material.

4.9 Vector spaces

Lemma 4.11. *If $\mathcal{V}$ is a subspace of $\mathbb{R}^n$ then* $\text{Span}(\mathcal{V}) = \mathcal{V}$.

Proof: Since $\mathcal{V}$ is a subspace, there exists a set $\mathcal{U}$ of vectors in $\mathbb{R}^n$ such that $\mathcal{V} = \text{Span}(\mathcal{U})$. Let $\vec{w}$ be a vector in $\text{Span}(\mathcal{V})$. Then $\vec{w}$ is a linear sum over $\mathcal{V}$; that is, there exists $\vec{v}_1 \ldots \vec{v}_q \in \mathcal{V}$ and scalars $a_1 \ldots a_k$ such that $\vec{w} = a_1\vec{v}_1 + \ldots + a_q\vec{v}_q$. Since $\mathcal{V} = \text{Span}(\mathcal{U})$, each of the $\vec{v}_i$ is a linear sum over $\mathcal{U}$; that is $\vec{v}_i = b_{i,1}\vec{u}_{i,1} + \ldots + b_{i,p}\vec{u}_{i,p}$ Thus

$$\vec{w} = a_1(b_{1,1}, \vec{u}_{1,1} + \ldots + b_{1,p}\vec{u}_{1,p}) + \ldots + a_q(b_{q,1}, \vec{u}_{q,1} + \ldots + b_{q,p}\vec{u}_{q,p}) = a_1b_{1,1}\vec{u}_{1,1} + \ldots + a_qb_{q,p}\vec{u}_{q,p}$$

Grouping together the repeated $\vec{u}$ vectors, we have an expression of $\vec{w}$ as a linear sum over $\mathcal{U}$. So $\vec{w}$ is in $\text{Span}(\mathcal{U}) = \mathcal{V}$. ∎

Theorem 4.12. *A set of n-dimensional vectors $\mathcal{V} \subset \mathbb{R}^n$ is a subspace of $\mathbb{R}^n$ if and only if it is closed under vector addition and scalar multiplication.*

Proof: Suppose $\mathcal{V}$ is a subspace of $\mathbb{R}^n$. By lemma 4.11, $\mathcal{V} = \text{Span}(\mathcal{V})$ so any linear sum of vectors in $\mathcal{V}$ is itself in $\mathcal{V}$. In particular if $\vec{v}$ and $\vec{u}$ are in $\mathcal{V}$ and a is a scalar, then $\vec{v} + \vec{u}$ and $a\vec{v}$ are in $\mathcal{V}$.

Conversely, suppose that $\mathcal{V}$ is closed under addition and scalar multiplication. Then if $\vec{w}$ is a linear sum over $\mathcal{V}$, $\vec{w} = a_1\vec{v}_1 + \ldots + a_q\vec{v}_q$, then each of the products $a_i\vec{v}_i$ is in $\mathcal{V}$, and then by induction, the partial sums

$$\begin{array}{l} a_1\vec{v}_1 + a_2\vec{v}_2, \\ a_1\vec{v}_1 + a_2\vec{v}_2 + a_3\vec{v}_3 \\ \ldots \\ a_1\vec{v}_1 + a_2\vec{v}_2 + \ldots + a_q\vec{v}_q \end{array}$$

are all in $\mathcal{V}$. So $\vec{w}$ is in $\mathcal{V}$. Since $\mathcal{V}$ contains all its linear sums, $\mathcal{V} = \text{Span}(\mathcal{V})$, so by definition 4.3, $\mathcal{V}$ is a subspace of $\mathbb{R}^n$. ∎

Lemma 4.13. *Let $\mathcal{V}$ be a set of n-dimensional vectors and let $\vec{w}$ be a vector in* $\text{Span}(\mathcal{V})$. *Then* $\text{Span}(\mathcal{V} \cup \{\vec{w}\}) = \text{Span}(\mathcal{V})$.

Proof: It is immediate that $\text{Span}(\mathcal{V} \cup \{\vec{w}\}) \supset \text{Span}(\mathcal{V})$, since any linear sum over $\mathcal{V}$ is a linear sum over $\mathcal{V} \cup \{\vec{w}\}$ with coefficient 0 on $\vec{w}$.

Since $\vec{w} \in \text{Span}(\mathcal{V})$ let $\vec{w} = a_1\vec{v}_1 + \ldots a_m\vec{v}_m$. Let $\vec{z}$ be any vector in $\text{Span}(\mathcal{V} \cup \{\vec{w}\})$. Then $\vec{z} = b_1\vec{v}_1 + \ldots + b_m\vec{v}_m + c\vec{w} = b_1\vec{z}_1 + \ldots b_m\vec{z}_m + c(a_1\vec{v}_1 + \ldots + a_m\vec{v}_m) = (b_1 + ca_1)\vec{z}_1 + \ldots + (b_m + ca_m)\vec{z}_m$. So $\vec{z}$ is a linear sum of $\vec{v}_1 \ldots \vec{v}_m$. ∎

4.10 Linear independence and bases

Theorem 4.14. *A set $\mathcal{V}$ is linearly dependent if and only if there exist distinct vectors $\vec{v}_1 \ldots \vec{v}_m$ in $\mathcal{V}$ and scalars $a_1 \ldots a_m$ which are not all equal to 0 such that $a_1\vec{v}_1 + \ldots a_m\vec{v}_m = \vec{0}$.*

Proof: Suppose that $\mathcal{V}$ is linearly dependent. Then by definition 4.4, there exists some $\vec{u}$ in $\mathcal{V}$ which is a linear sum over the other vectors in $\mathcal{V}$; that is, $\vec{u} = a_1\vec{v}_1 + \ldots + a_m\vec{v}_m$. Therefore $\vec{0} = a_1\vec{v}_1 + \ldots + a_m\vec{v}_m - \vec{u}$. Note that the coefficient of $\vec{v}$ is -1, so the coefficients in this sum are not all zero, satisfying the condition of the theorem.

Conversely, suppose that $\mathcal{V}$ satisfies the conditions of the theorem; that is $a_1\vec{v}_1 + \ldots a_m\vec{v}_m = \vec{0}$, where the coefficients are not all 0. Let a_i be some non-zero coefficient. Then, we can solve for $\vec{v}_i$ in the above equation

$$\vec{v}_i = -\frac{a_1}{a_i}\vec{v}_1 - \ldots - \frac{a_{i-1}}{a_i}\vec{v}_{i-1} - \frac{a_{i+1}}{a_i}\vec{v}_{i+1} - \ldots - \frac{a_m}{a_i}\vec{v}_m$$

so $\vec{v}_i$ is a linear sum of the rest of the vectors. ∎.

Corollary 4.15. *Let $\vec{v}_1, \vec{v}_2 \ldots \vec{v}_k$ be a sequence of vectors such that for all i, $\vec{v}_i$ is not in Span($\{\vec{v}_1 \ldots \vec{v}_{i-1}\}$). Then $\vec{v}_1, \vec{v}_2 \ldots \vec{v}_k$ are linearly independent.*

Proof of the contrapositive: Suppose that $\vec{v}_1, \vec{v}_2 \ldots \vec{v}_k$ are linearly dependent. Then for some $a_1 \ldots a_k$ not all zero, $a_1\vec{v}_1 + \ldots + a_k\vec{v}_k = \vec{0}$. Let i be the largest index for which $a_i \neq 0$. Then $\vec{v}_i = (-1/a_i)(a_1\vec{v}_1 + \ldots + a_{i-1}\vec{v}_{i-1})$, so $\vec{v}_p$ is in Span($\{\vec{v}_1 \ldots \vec{v}_{i-1}\}$). ∎

Theorem 4.16. *If $\mathcal{B} = \langle\vec{b}_1 \ldots \vec{b}_m\rangle$ is a basis for $\mathcal{V}$, then any vector $\vec{v}$ in $\mathcal{V}$ has a unique tuple of coordinates relative to $\mathcal{B}$. That is, there is a unique sequence of coefficients $a_1 \ldots a_m$ such that $\vec{v} = a_1\vec{b}_1 + \ldots + a_m\vec{b}_m$.*

Proof: The fact that there exist such an $a_1 \ldots a_m$ is immediate from the fact that $\vec{v} \in$Span($\mathcal{B}$). To prove that the coordinate vector is unique, suppose that $\vec{v} = a_1\vec{b}_1 + \ldots + a_m\vec{b}_m = c_1\vec{b}_1 + \ldots + c_m\vec{b}_m$. Then $(a_1 - c_1)\vec{b}_1 + \ldots + (a_m - c_m)\vec{b}_m = \vec{0}$. Since the $\vec{b}_i$ are linearly independent, $a_i - c_i = 0$ for all i. ∎

Lemma 4.17. *Let $\mathcal{B} = \{\vec{b}_1 \ldots \vec{b}_m\}$ be a set of linearly independent n-dimensional vectors. Let $\mathcal{V} = \vec{v}_1 \ldots \vec{v}_p$ be a set of linearly independent vectors in* Span($\mathcal{B}$). *Then $p \leq m$.*

Proof: Since $\vec{v}_1 \in$ Span($\mathcal{B}$), we can write $\vec{v}_1 = a_1\vec{b}_1 + \ldots + a_m\vec{b}_m$ where one of the coefficients a_i is non-zero. Since the numbering on the b vectors does not matter, we can renumber them so that the coefficient a_1 is non-zero. (This renumbering is not significant; it just simplifies the wording of the proof.) Then we can solve for $\vec{b}_1$ and write

$$\vec{b}_1 = \frac{1}{a_1}\vec{v}_1 - \frac{a_2}{a_1}\vec{b}_2 - \ldots - \frac{a_m}{a_1}\vec{b}_m$$

Thus $\vec{b}_1$ is in Span($\vec{v}_1, \vec{b}_2, \ldots \vec{b}_m$) so by lemma 4.13 Span($\vec{v}_1, \vec{b}_2, \ldots \vec{b}_m$) = Span($\mathcal{B} \cup \{\vec{v}_1\}$) = Span($\mathcal{B}$).

Moving on, we have $\vec{v}_2 \in$ Span($\mathcal{B}$); so $\vec{v}_2$ is in Span($\vec{v}_1, \vec{b}_2, \ldots \vec{b}_m$); so $\vec{v}_2 = c_1\vec{v}_1 + c_2\vec{b}_2 + \ldots + c_m\vec{b}_m$. Since $\vec{v}_2$ and $\vec{v}_1$ are linearly independent, it cannot be the case that c_1 is the only non-zero coefficient; at least one of the coefficients associated with $\vec{b}_2 \ldots \vec{b}_m$ must be non-zero. Again by renumbering we can assume that that is c_2. Again, we can solve for $\vec{b}_2$ and show that $\vec{b}_2$ is a linear sum of $\vec{v}_1, \vec{v}_2, \vec{b}_3 \ldots \vec{b}_m$. We now have that Span($\vec{v}_1, \vec{v}_2, \vec{b}_3, \ldots \vec{b}_m$) = Span($\mathcal{B}$).

We can keep doing this, replacing a vector in $\mathcal{B}$ with vector $\vec{v}_i$ while maintaining the same span, until either we have moved all the $\vec{v}$ vectors into the set, if $p < m$, or we have replaced all the $\vec{b}$ vectors, if $p \geq m$. Now suppose that $p > m$. At this point we have Span($\vec{v}_1 \ldots \vec{v}_m$) = Span($\mathcal{B}$) so for $i = m + 1 \ldots p$, $\vec{v}_i$ is in Span($\vec{v}_1 \ldots \vec{v}_m$). But that contradicts the assumption that $\vec{v}_1 \ldots \vec{v}_p$ are linearly independent. Therefore we must have $p \leq m$. ∎

Corollary 4.18. *Any two bases for the same vector space have the same number of vectors.*

Proof: Let $\mathcal{B}$ and $\mathcal{C}$ be bases for vector space $\mathcal{V}$. Let m be the number of vectors in $\mathcal{B}$. By lemma 4.17, since $\mathcal{C}$ is linearly independent, it cannot have more than m vectors. Since neither basis can have more vectors than the other, they must have equal numbers. ∎

Corollary 4.19. *A set of linearly independent vectors in $\mathbb{R}^n$ has at most n vectors.*

Proof: Immediate from lemma 4.17 and the fact that $\{\vec{e}^{\,1} \ldots \vec{e}^{\,n}\}$ is a basis for $\mathbb{R}^n$.

The number of vectors in a basis for vector space $\mathcal{V}$ is called the *dimension* of $\mathcal{V}$, denoted "Dim($\mathcal{V}$)". By convention, the dimension of the zero space is zero.

Lemma 4.20. *Let $\mathcal{B}$ be a linearly independent set of n-dimensional vectors. If $\vec{v}$ is not a linear sum of $\mathcal{B}$, then $\mathcal{B} \cup \{\vec{v}\}$ is linearly independent.*

Proof of the contrapositive. Suppose that $\mathcal{B}$ is linearly independent and $\mathcal{B} \cup \{\vec{v}\}$ is not. Then there exist scalars $a_0 \ldots a_m$, not all zero, such that $a_1\vec{b}_1 + \ldots + a_m\vec{b}_m + a_0\vec{v} = \vec{0}$. Since $\vec{b}_1 \ldots \vec{b}_m$ are linearly independent, a_0 cannot be 0. Therefore we can solve for $\vec{v}$,

$$\vec{v} = -\frac{a_1}{a_0}\vec{b}_1 \ldots - \frac{a_m}{a_0}\vec{b}_m$$

so $\vec{v}$ is a linear sum of $\vec{b}_1 \ldots \vec{b}_m$.

Theorem 4.21. *Let $\mathcal{V}$ be a subspace of $\mathbb{R}^n$ and let $\mathcal{U}$ be a set of linearly independent vectors in $\mathcal{V}$. Then $\mathcal{U}$ can be extended to a basis for $\mathcal{V}$; that is, there exists a basis $\mathcal{B}$ for $\mathcal{V}$ such that $\mathcal{U} \subset \mathcal{B}$.*

Proof: If Span($\mathcal{U}$) = $\mathcal{V}$, then choose $\mathcal{B} = \mathcal{U}$. Otherwise, let $\vec{v}_1$ be a vector in $\mathcal{V}$ that is not in Span($\mathcal{U}$). Let $\mathcal{U}_1 = \mathcal{U} \cup \{\vec{v}_1\}$. By lemma 4.20 $\mathcal{U}_1$ is linearly independent. Clearly Span($\mathcal{U}_1$) $\subset \mathcal{V}$.

If Span($\mathcal{U}_1$) = $\mathcal{V}$ then we are done. If not, then we choose a vector $\vec{v}_2$ in $\mathcal{V} - (\mathcal{U} \cup \{\vec{v}_1\})$ and let $\mathcal{U}_2 = \mathcal{U}_1 \cup \{\vec{v}_2\}$. We can keep doing this until Span($\mathcal{U}_k$) = $\mathcal{V}$ for some k. Certainly it will have to stop before $\mathcal{U}_k$ gets more than n vectors, since there cannot be more than n linearly independent n-dimensional vectors. ∎

Corollary 4.22. *Any subspace of $\mathbb{R}^n$ has a basis.*

Proof: By theorem 4.21, the empty set of vectors can be extended to a basis.

Corollary 4.23. *Let $\mathcal{V}$ be a vector space of dimension m. Any set $\mathcal{B}$ of m linearly independent vectors in $\mathcal{V}$ spans $\mathcal{V}$ and thus is a basis for $\mathcal{V}$.*

Proof: By theorem 4.21 $\mathcal{B}$ can be extended to a basis for $\mathcal{V}$. By corollary 4.18 this extension must have m vectors; thus, it must be equal to $\mathcal{B}$.

Theorem 4.24. *Let $\mathcal{V}$ be a vector space of dimension m, and let $\mathcal{B} = \{\vec{b}_1 \ldots \vec{b}_p\}$ be a finite set of vectors that spans $\mathcal{V}$. Then $p \geq m$, and there exists a subset of $\mathcal{B}$ which is a basis for $\mathcal{V}$.*

Proof: If $\mathcal{B}$ is linearly independent, then it is a basis for $\mathcal{V}$, so by corollary 4.18 $p = m$.

If $\mathcal{B}$ is not linearly independent, then let $\vec{v}$ be a vector in $\mathcal{B}$ which is the linear sum of other vectors in $\mathcal{B}$. It is immediate that we can delete $\vec{v}$; that is, $\mathcal{B} - \{\vec{v}\}$ still spans $\mathcal{V}$. If the result is still not linearly independent we can repeat this. Eventually, we will reach a subset of $\mathcal{B}$ which is linearly independent and which still spans $\mathcal{V}$. This is a subset of $\mathcal{B}$ which is a basis for $\mathcal{V}$, and so must contain m vectors. ∎

4.11 Sum of vector spaces

Throughout this section, let $\mathcal{U}$ and $\mathcal{V}$ be subspaces of $\mathbb{R}^n$.

Theorem 4.25. *The direct sum $\mathcal{U} \oplus \mathcal{V}$ and the intersection $\mathcal{U} \cap \mathcal{V}$ are vector spaces.*

Proof: Immediate from the definitions.

Theorem 4.26. $\text{Dim}(\mathcal{U}) \oplus \text{Dim}(\mathcal{V}) = \text{Dim}(\mathcal{U}) + \text{Dim}(\mathcal{V}) - \text{Dim}(\mathcal{U} \cap \mathcal{V})$

Proof: Let $p = \text{Dim}(\mathcal{U})$, $q = \text{Dim}(\mathcal{V})$, $r = \text{Dim}(\mathcal{U} \cap \mathcal{V})$. Clearly $r \leq p$ and $r \leq q$. Let $\mathcal{W} = \{\vec{w}_1 \ldots \vec{w}_r\}$ be a basis for $\mathcal{U} \cap \mathcal{V}$. Using theorem 4.21, let $\mathcal{B} = \{\vec{b}_1 \ldots \vec{b}_{p-r}\}$ be a set of vectors such that $\mathcal{W} \cup \mathcal{B}$ is a basis for $\mathcal{U}$; and let $\mathcal{C} = \{\vec{c}_1 \ldots \vec{c}_{q-r}\}$ be a set of vectors such that $\mathcal{W} \cup \mathcal{C}$ is a basis for $\mathcal{V}$. (If $p = r$ then let $\mathcal{B} = \emptyset$; if $q = r$ then let $\mathcal{C} = \emptyset$.)

Let $\mathcal{Q} = \mathcal{W} \cup \mathcal{B} \cup \mathcal{C}$. I claim that $\mathcal{Q}$ is a basis for $\mathcal{U} \oplus \mathcal{V}$. To prove this we must show that $\mathcal{Q}$ spans $\mathcal{U} \oplus \mathcal{V}$ and that $\mathcal{Q}$ is linearly independent.

Since every vector in $\mathcal{U} \oplus \mathcal{V}$ is a linear sum over $\mathcal{U} \cup \mathcal{V}$, every vector in $\mathcal{U}$ is a linear sum over $\mathcal{W} \cup \mathcal{B}$ and every vector in $\mathcal{V}$ is a linear sum over $\mathcal{W} \cup \mathcal{C}$, it follows that $\mathcal{U} \oplus \mathcal{V} = \text{Span}(\mathcal{Q})$.

To show that $\mathcal{Q}$ is linearly independent, suppose that
$a_1\vec{w}_1 + \ldots + a_r\vec{w}_r + d_1\vec{b}_1 + \ldots + d_{p-r}\vec{b}_{p-r} + e_1\vec{c}_1 + \ldots + e_{q-r}\vec{c}_{q-r} = \vec{0}$. Then
$a_1\vec{w}_1 + \ldots + a_r\vec{w}_r + d_1\vec{b}_1 + \ldots + d_{p-r}\vec{b}_{p-r} = -e_1\vec{c}_1 + \ldots + -e_{q-r}\vec{c}_{q-r}$.
But the left hand side is a vector in $\mathcal{U}$ and the right hand side is a vector in $\text{Span}(\mathcal{C})$. Let us call this vector $\vec{z}$. Then $\vec{z} \in \text{Span}(\mathcal{C}) \cap \mathcal{U}$, so $\vec{z} \in \mathcal{U} \cap \mathcal{V}$. But the vectors in $\mathcal{C}$ are linearly independent of those in $\mathcal{U} \cap \mathcal{V}$; hence $\vec{z} = \vec{0}$. Therefore, all the coefficients a_i, d_i and e_i are equal to 0. ∎

Theorem 4.27. *Every subspace $\mathcal{V}$ of $\mathbb{R}^n$ has a complement.*

Proof: Using corollary 4.22, let $\mathcal{B}$ be a basis for $\mathcal{V}$. Using theorem 4.21, let $\mathcal{Q}$ be an extension of $\mathcal{B}$ to a basis for $\mathbb{R}^n$. It is easily shown that $\text{Span}(\mathcal{Q} \setminus \mathcal{B})$ is a complement for $\mathcal{V}$. ∎

4.12 Orthogonality

Recall that two vectors are *orthogonal* if their dot product is equal to 0.

Definition 4.6. *Let $\mathcal{U}$ and $\mathcal{V}$ be subspaces of $\mathbb{R}^n$. $\mathcal{U}$ and $\mathcal{V}$ are* orthogonal *if, for every $\vec{u}$ in $\mathcal{U}$ and $\vec{v}$ in $\mathcal{V}$, $\vec{u}$ is orthogonal to $\vec{v}$.*

$\mathcal{U}$ and $\mathcal{V}$ are orthogonal complements *if they are orthogonal and they are complements.*

A finite set $\mathcal{B} = \vec{b}_1 \ldots \vec{b}_q$ is orthogonal *if, for $i \neq j$, $\vec{b}_i$ is orthogonal to $\vec{b}_j$.*

An orthogonal basis *for subspace $\mathcal{V}$ is a basis for $\mathcal{V}$ that is orthogonal.*

Theorem 4.28. *Let $\mathcal{V}$ be a vector space and let $\mathcal{B}$ be an orthonormal basis for V. Then:*

- *For any $\vec{u}, \vec{w} \in \mathcal{V}$, $\vec{u} \bullet \vec{w} = \text{Coords}(\vec{u}, \mathcal{B}) \bullet \text{Coords}(\vec{w}, \mathcal{B})$.*
- *For any $\vec{u} \in \mathcal{V}$, $|\vec{u}| = |\text{Coords}(\vec{u}, \mathcal{B})|$.*

Proof: Let $\mathcal{B} = \{\hat{b}_1 \ldots \hat{b}_m\}$. Let $\text{Coords}(\vec{u}, \mathcal{B}) = \langle u_1 \ldots u_m \rangle$ and let $\text{Coords}(\vec{v}, \mathcal{B}) = \langle v_1 \ldots v_m \rangle$. Then

$$\vec{u} \bullet \vec{v} = (u_1 \cdot \hat{b}_1 + \ldots + u_m \cdot \hat{b}_m) \bullet (v_1 \cdot \hat{b}_1 + \ldots + v_m \cdot \hat{b}_m) =$$

$$u_1 \cdot v_1 \cdot (\hat{b}_1 \bullet \hat{b}_1) + u_1 \cdot v_2 \cdot (\hat{b}_1 \bullet \hat{b}_2) + \ldots + u_1 \cdot v_m \cdot (\hat{b}_1 \bullet \hat{b}_m) +$$
$$u_2 \cdot v_1 \cdot (\hat{b}_2 \bullet \hat{b}_1) + \ldots + u_2 \cdot v_m \cdot (\hat{b}_2 \bullet \hat{b}_m) +$$
$$\ldots$$
$$+u_m \cdot v_1 \cdot (\hat{b}_m \bullet \hat{b}_1) + \ldots + u_m \cdot v_m \cdot (\hat{b}_m \bullet \hat{b}_m)$$

But since $\mathcal{B}$ is orthonormal the dot product $\hat{b}_i \bullet \hat{b}_j$ is equal to 0 if $i \neq j$ and are equal to 1 if $i = j$. Therefore, the above sum boils down to

$$u_1 \cdot v_1 + u_2 \cdot v_2 + \ldots + u_m \cdot v_m = \text{Coords}(\vec{u}, \mathcal{B}) \bullet \text{Coords}(\vec{v}, \mathcal{B})$$

For the second part of the theorem, note that

$$|\vec{u}| = \sqrt{\vec{u} \bullet \vec{u}} = \sqrt{\text{Coords}(\vec{u}, \mathcal{B}) \bullet \text{Coords}(\vec{u}, \mathcal{B})} = |\text{Coords}(\vec{u}, \mathcal{B})|$$

∎

Theorem 4.29. *Let $\mathcal{B} = \{\vec{b}_1 \ldots \vec{b}_q\}$ be an orthonormal basis for vector space $\mathcal{V}$. If $\vec{v}$ is a vector in $\mathcal{V}$, then the ith coordinate of $\vec{v}$ with respect to $\mathcal{B}$,* $\text{Coords}(\vec{v}, \mathcal{B})[i] = \vec{v} \bullet \vec{b}_i$.

Proof: Let $c_i = \text{Coords}(\vec{v}, \mathcal{B})[i]$. Then $\vec{v} = c_1\vec{b}_1 + \ldots + c_q\vec{b}_q$, by definition of Coords. So

$$\vec{v} \bullet \vec{b}_i = (c_1\vec{b}_1 + \ldots + c_q\vec{b}_q) \bullet \vec{b}_i = c_1(\vec{b}_1 \bullet \vec{b}_i) + \ldots + c_q(\vec{b}_q \bullet \vec{b}_i) = c_i$$

because $\vec{b}_i \bullet \vec{b}_i = 1$ and $\vec{b}_i \bullet \vec{b}_j = 0$ for $j \neq i$. ∎

Definition 4.7. *Let $\mathcal{B} = \vec{b}_1 \ldots \vec{b}_q$ be an orthogonal set of n-dimensional vectors, and let $\vec{v}$ be an n-dimensional vector.*

Define $\text{Project}(\vec{v}, \mathcal{B})$ *as*

$$\text{Project}(\vec{v}, \mathcal{B}) = \frac{\vec{v} \bullet \vec{b}_1}{\vec{b}_1 \bullet \vec{b}_1} \cdot \vec{b}_1 + \ldots + \frac{\vec{v} \bullet \vec{b}_q}{\vec{b}_q \bullet \vec{b}_q} \cdot \vec{b}_q$$

Note that $\text{Project}(\vec{v}, \mathcal{B})$ is in $\text{Span}(\mathcal{B})$. As we shall see in chapter 6, $\text{Project}(\vec{v}, \mathcal{B})$ is in fact the point in $\text{Span}(\mathcal{B})$ that is closest to $\vec{v}$.

Lemma 4.30. *Let $\mathcal{B} = \vec{b}_1 \ldots \vec{b}_q$ be an orthogonal set of n-dimensional vectors, and let $\vec{v}$ be an n-dimensional vector that is not in* $\text{Span}(\mathcal{B})$. *Let $\vec{u} = \vec{v} - \text{Project}(\vec{v}, \mathcal{B})$; note that $\vec{u}$ is in* $\text{Span}(\mathcal{B} \cup \{\vec{v}\})$. *Then $\vec{u}$ is orthogonal to $\vec{b}_1 \ldots \vec{b}_q$.*

Proof: For any i,

$$\vec{u} \bullet \vec{b}_i = (\vec{v} - \frac{\vec{v} \bullet \vec{b}_1}{\vec{b}_1 \bullet \vec{b}_1} \cdot \vec{b}_1 - \ldots - \frac{\vec{v} \bullet \vec{b}_q}{\vec{b}_q \bullet \vec{b}_q} \cdot \vec{b}_q) \bullet \vec{b}_i = \vec{v} \bullet \vec{b}_i - \frac{\vec{v} \bullet \vec{b}_1}{\vec{b}_1 \bullet \vec{b}_1} \cdot \vec{b}_1 \bullet \vec{b}_i - \ldots - \frac{\vec{v} \bullet \vec{b}_q}{\vec{b}_q \bullet \vec{b}_q} \cdot \vec{b}_q \bullet \vec{b}_i$$

Since the $\vec{b}$'s are orthogonal, $\vec{b}_j \bullet \vec{b}_i = 0$ for all $j \neq i$, so all these terms disappear except

$$\vec{v} \bullet \vec{b}_i - \frac{\vec{v} \bullet \vec{b}_i}{\vec{b}_i \bullet \vec{b}_i} \cdot \vec{b}_i \bullet \vec{b}_i = 0$$

∎

Theorem 4.31. *Any vector space $\mathcal{V}$ has an orthogonal basis and an orthogonal complement.*

Proof: Carry out the following procedure:

{ let $\mathcal{C} = \{\vec{c}_1 \dots \vec{c}_q\}$ be any basis for $\mathcal{V}$;
  extend $\mathcal{C}$ to a basis $\{\vec{c}_1 \dots \vec{c}_n\}$ for $\mathbb{R}^n$;
  $\mathcal{B} = \emptyset$;
  $\mathcal{D} = \emptyset$;
  for $(i = 1 \dots q)$ {
    let $\vec{u}_i = \vec{c}_i - \text{Project}(\vec{c}_i, \mathcal{B})$;
    add $\vec{u}_i$ to $\mathcal{B}$; }
  for $(i = q+1 \dots n)$ {
    let $\vec{u}_i = \vec{c}_i - \text{Project}(\vec{c}_i, \mathcal{B} \cup \mathcal{D})$;
    add $\vec{u}_i$ to $\mathcal{D}$; }
}

It then immediate from lemma 4.30 that $\mathcal{B}$ is an orthogonal basis for $\mathcal{V}$ and that Span($\mathcal{D}$) is the orthogonal complement for $\mathcal{V}$. ∎

This procedure is known as *Gram-Schmidt orthogonalization.*

Example 4.12: In $\mathbb{R}^4$, let $\mathcal{C}$ be the set of two vectors $\langle 1,1,1,1\rangle$ $\langle 0,0,1,1\rangle$. Extend $\mathcal{B}$ to a basis for $\mathbb{R}^4$ by adding the two vectors $\vec{e}^{\,1}, \vec{e}^{\,3}$. Then

$\vec{u}_1 = \vec{c}_1 = \langle 1,1,1,1\rangle$
$\vec{u}_2 = \vec{c}_2 - \frac{\vec{u}_1 \bullet \vec{c}_2}{\vec{u}_1 \bullet \vec{u}_1} \cdot \vec{u}_1 = \langle 0,0,1,1\rangle \; - \; \frac{2}{4} \cdot \langle 1,1,1,1\rangle = \langle -1/2, -1/2, 1/2, 1/2\rangle$
$\mathcal{B} = \{\vec{u}_1, \vec{u}_2\}$.
$\vec{u}_3 = \vec{c}_3 - \frac{\vec{u}_1 \bullet \vec{c}_3}{\vec{u}_1 \bullet \vec{u}_1} \cdot \vec{u}_1 - \frac{\vec{u}_2 \bullet \vec{c}_3}{\vec{u}_2 \bullet \vec{u}_2} \cdot \vec{u}_2 =$
  $\langle 1,0,0,0\rangle \; - \; \frac{1}{4}\langle 1,1,1,1\rangle \; - \; \frac{-1/2}{1}\langle -1/2, -1/2, 1/2, 1/2\rangle =$
  $\langle 1/2, -1/2, 0, 0\rangle$.
$\vec{u}_4 = \vec{c}_4 - \frac{\vec{u}_1 \bullet \vec{c}_4}{\vec{u}_1 \bullet \vec{u}_1} \cdot \vec{u}_1 - \frac{\vec{u}_2 \bullet \vec{c}_4}{\vec{u}_2 \bullet \vec{u}_2} \cdot \vec{u}_2 - \frac{\vec{u}_3 \bullet \vec{c}_4}{\vec{u}_3 \bullet \vec{u}_3} \cdot \vec{u}_3 =$
  $\langle 0,0,1,0\rangle \; - \; \frac{1}{4}\langle 1,1,1,1\rangle \; - \frac{1/2}{1}\langle -1/2, -1/2, 1/2, 1/2\rangle \; - \; \frac{0}{1/2}\langle 1/2, -1/2, 0, 0\rangle =$
  $\langle 0,0,1/2, -1/2\rangle$
$\mathcal{D} = \{\vec{u}_3, \vec{u}_4\}$.

Corollary 4.32. *The set of all vectors orthogonal to $\mathcal{V}$ is complementary to $\mathcal{V}$ and is therefore the orthogonal complement of $\mathcal{V}$.*

Proof: Clearly any vector orthogonal to $\mathcal{V}$ is in the orthogonal complement of $\mathcal{V}$ and vice versa. What is non-trivial here is that there exists an orthogonal complement, which is guaranteed by theorem 4.31.

4.13 Functions

We now turn to linear transformations, but we begin with some simple observations about functions in general, from any domain to any range.

Definition 4.8. *Let f be a function from domain D to range E. Let S be a subset of D. Then $f(S) = \{f(s) | s \in S\}$, the set of values obtained by applying f to elements of S. We define* Image$(f) = f(D)$*, the set of values obtained by applying f to any element in the domain D.*

Definition 4.9. *Let f be a function from domain D to range E. Let S be a subset of D and let T be a subset of E. We say that f is a* surjection *from S onto T (or "f maps S onto T") if T is a subset of Image(f). We say that f is an* injection *over S (or "f is one-to-one on S") if f maps each element of S to a different element of E; that is, if s_1, s_2 are in S and $s_1 \neq s_2$ then $f(s_1) \neq f(s_2)$. We say that f is a* bijection *from S to T, if $f(S) = T$ and f is an injection over S.*

Definition 4.10. *Let f be a function from D to E, and let g be a function from E to D. Suppose that, for every element d of D, $g(f(d)) = d$. Then we say that g is a* left inverse *of f and that f is a* right inverse *of g.*

Example 4.13: Let $D = \{a, b, c\}$ and let $E = \{1, 2, 3, 4\}$. The function $f : D \rightarrow E$ defined by $f(a) = 4, f(b) = 2, f(c) = 3$ is an injection. The function $g : D \rightarrow E$ defined by $g(a) = 4, g(b) = 2, g(c) = 4$ is not an injection because $g(a) = g(c)$. There obviously cannot be a surjection from D to E, because there are more elements in E than D. The function $j : E \rightarrow D$ defined by $j(1) = b, j(2) = b, j(3) = c, j(4) = a$ is a surjection. The function $h : E \rightarrow D$ defined by $h(1) = a, h(2) = b, h(3) = b, h(4) = a$ is not a surjection, because there is no value x such that $j(x) = c$. There cannot be an injection from E to D because there are more elements in E than in D; this is known as the *pigeon-hole principle.*

Image(f) $= \{2, 3, 4\}$. Image(g) $= \{2, 4\}$. Image(j) $= \{a, b, c\}$. Image(h) $= \{a, b\}$.

Function j is a left inverse of f and f is a right inverse of j because $j(f(a)) = j(4) = a$; $j(f(b)) = j(2) = b$, and $j(f(c)) = j(3) = c$.

Example 4.14: Consider functions from $\mathbb{Z}$, the set of integers, to itself. The function $f(x) = 2x$ is an injection – if $2x = 2y$ then $x = y$ – but not a surjection — if z is odd, then there is no x such that $f(x) = z$. The function $g(x) = \lfloor x/2 \rfloor$ is a surjection — for any z, $g(2z) = z$ and $g(2z + 1) = z$ — but not an injection — for any z, $g(2z) = g(2z + 1)$. Image(f) is the set of all even integers. Image(g) is the set of all integers. Function g is a left inverse of f, and f is a right inverse of g.

Example 4.15: Of course, the case that actually interests us here is linear transformations. Let $D = \mathbb{R}^3$ and let $E = \mathbb{R}^2$. Let $f : D \rightarrow E$ be the function

$$f(\vec{v}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \cdot \vec{v}$$

Function f is a surjection because for any vector $\langle x, y \rangle \in E$, $f(\langle x, y, 0 \rangle) = \langle x, y \rangle$. It is not an injection because $f(\langle x, y, 1 \rangle) = f(\langle x, y, 0 \rangle) = \langle x, y \rangle$.

Let $g : D \rightarrow E$ be the function

$$g(\vec{v}) = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \cdot \vec{v}$$

Function g is not a surjection because for any vector $\langle x, y, z \rangle \in D$, $g(\langle x, y, z \rangle) = \langle x, x \rangle$, so for any $y \neq x$, the vector $\langle x, y \rangle$ is not in Image(g). Nor is g an injection.

Let $h : E \rightarrow D$ be the function

$$h(\vec{v}) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{bmatrix} \cdot \vec{v}$$

Function h is a injection because, if $h(\langle w, x \rangle) = h(\langle y, z \rangle)$ then we have $h(\langle w, x \rangle) = \langle w, x, w + x \rangle$ and $h(\langle y, z \rangle) = \langle y, z, y + z \rangle$ so $w = y$ and $x = z$. It is not an surjection because for any vector $\langle x, y, z \rangle \in D$, if $z \neq x + y$ then $\langle x, y, z \rangle$ is not in Image(f).

Let $j : E \rightarrow D$ be the function

$$j(\vec{v}) = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \end{bmatrix} \cdot \vec{v}$$

Function j is not an injection because, $h(\langle 4,2\rangle) = h(\langle 4,5\rangle) = \langle 4,4,4\rangle$. It is certainly not a surjection.

Function h is a right inverse for f, and f is a left inverse for h, because, for any vector $\langle x,y\rangle$ in E,

$$f(h(\langle x,y\rangle)) = f(\langle x,y,x+y\rangle) = \langle x,y\rangle$$

Not coincidentally, the corresponding matrix product is the identity.

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Theorem 4.33. *If g is a left inverse for f, then f is an injection over D and g is a surjection onto D.*

Proof: Assume g is a left inverse for f; then $g(f(d)) = d$ for all d in D. Then for every d in D there exists r in E for which $g(r) = d$; namely $r = f(d)$. Thus g is a surjection onto D.

If f is not an injection then there exists d and e in D such that $d \neq e$ but $f(d) = f(e)$. Since $g(f(d)) = g(f(e))$ we cannot have both $g(f(d)) = d$ and $g(f(e)) = e$. ∎

Definition 4.11. *If g is both a left inverse and a right inverse for f, then g is said to be the* full inverse *or simply the* inverse *of f. We write $g = f^{-1}$. (Note that there can only exist one inverse.)*

Theorem 4.34. *Function f has an inverse if and only if f is a bijection.*

Proof: By theorem 4.33, if f has an inverse then f is a bijection. Conversely, if f is a bijection then, for each r in E there is a unique d in D for which $f(d) = r$; we define the inverse g such that $g(r) = d$. ∎

Theorem 4.35. *If g is a left inverse of f and h is a right inverse of f, then $g = h$ and $g = f^{-1}$.*

Proof: Let i_D be the identity function over D and let i_E be the identity function over E. Then $g = g \circ i_E = g \circ (f \circ h) = (g \circ f) \circ h = i_D \circ h = h$. ∎

If that seems so clever as to be suspicious, you can write it out long-hand as follows. Let e be any element of E and consider $g(f(h(e)))$. On the one hand, since h is the right inverse of f, $f(h(e)) = e$ so $g(f(h(e))) = g(e)$. On the other hand since g is the left inverse of f, $g(f(d)) = d$ for all d in D. In particular, this holds for $d = h(e)$. Thus $g(f(h(e))) = h(e)$. Thus for all e in E, $g(r) = g(f(h(e))) = h(e)$. Since g and h have the same value for all arguments, they are the same function.

4.14 Linear transformations

We now return to linear transformations. For the remainder of this section, $f(\vec{v})$ will be a linear transformation from $\mathbb{R}^n$ to $\mathbb{R}^m$, and F will be the corresponding matrix.

Theorem 4.36. *For any linear mapping f from $\mathbb{R}^n$ to $\mathbb{R}^m$,* Image(f) *and* Null(f) *are vector spaces. Thus* Image(f) *is a subspace of $\mathbb{R}^m$ and* Null(f) *is a subspace of $\mathbb{R}^n$.*

Proof: We leave this as an exercise (Problem 4.4).

Theorem 4.37. *For any finite set of n-dimensional vectors, $\mathcal{B}$,* Span$(f(\mathcal{B})) = f($Span$(\mathcal{B}))$

Proof: Immediate from the fact that $f(a_1\vec{b}_1 + \ldots + a_q\vec{b}_q) = a_1 f(\vec{b}_1) + \ldots + a_q f(\vec{b}_q)$.

Corollary 4.38. *For any subspace $\mathcal{V}$ of $\mathbb{R}^n$, $\mathrm{Dim}(f(\mathcal{V})) \leq \min(m, \mathrm{Dim}(\mathcal{V}))$. In particular, $\mathrm{Rank}(f) \leq \min(m, n)$.*

Proof: Since $f(\mathcal{V})$ is a subset of $\mathbb{R}^m$ it follows that $\mathrm{Dim}(\mathcal{V}) \leq m$.

Let $\vec{b}_1 \ldots \vec{b}_q$ be a basis for $\mathcal{V}$, where $q = \mathrm{Dim}(\mathcal{V})$. Then by theorem 4.37, $f(\vec{b}_1) \ldots f(\vec{b}_q)$ spans $f(\mathcal{V})$ (they may not be linearly independent). Hence, by theorem 4.24, $\mathrm{Dim}(f(\mathcal{V})) \leq q$.

For the second statement, we have $\mathrm{Rank}(f) = \mathrm{Dim}(f(\mathcal{V}))$ where $\mathcal{V} = \mathbb{R}^n$, so $\mathrm{Rank}(f) = \mathrm{Dim}(f(\mathbb{R}^n)) \leq \mathrm{Dim}(\mathbb{R}^n) = n$. ∎

Theorem 4.39. *Let $\mathcal{B}$ be a linearly independent set, and let $\mathcal{V} = \mathrm{Span}(\mathcal{B})$. If f is an injection over $\mathcal{V}$ then $f(\mathcal{B})$ is a linearly independent set.*

Proof of the contrapositive. Suppose that f is an injection and $f(\mathcal{B})$ is linearly dependent. Let $\mathcal{B} = \{\vec{b}_1 \ldots \vec{b}_q\}$. Then for some $a_1 \ldots a_q$ not all equal to 0, $\vec{0} = a_1 f(\vec{b}_1) + \ldots + a_q f(\vec{b}_q) = f(a_1\vec{b}_1 + \ldots a_q\vec{v}_q)$. Since $\vec{0} = f(\vec{0})$ and f is an injection we must have $a_1\vec{b}_1 + \ldots a_q\vec{b}_q = \vec{0}$, so $\vec{b}_1 \ldots \vec{b}_q$ are linearly dependent. ∎

Corollary 4.40. *If f has a left inverse, then $m \geq n$.*

Proof: By theorem 4.33, if f has a left inverse, then f is an injection. Let $\mathcal{B}$ be a basis for $\mathbb{R}^n$. By theorem 4.39, $f(\mathcal{B})$, which is a set of vectors in $\mathbb{R}^m$, is linearly independent, so by corollary 4.19 $n \leq m$.

Theorem 4.41. *Let $\mathcal{V}$ be a complement to* $\mathrm{Null}(f)$*. Then f is a bijection between $\mathcal{V}$ and* $\mathrm{Image}(f)$*.*

Proof: Let $\vec{u}$ be any vector in $\mathrm{Image}(f)$; thus $\vec{u} = f(\vec{w})$ for some $\vec{w}$ in $\mathbb{R}^n$. Since $\mathcal{V}$ is a complement of $\mathrm{Null}(f)$, we have $\vec{w} = \vec{v} + \vec{n}$ for some $\vec{v}$ in $\mathcal{V}$ and some $\vec{n}$ in $\mathrm{Null}(f)$. Then $\vec{u} = f(\vec{w}) = f(\vec{v} + \vec{n}) = f(\vec{v}) + f(\vec{n}) = f(\vec{v}) + \vec{0} = f(\vec{v})$ so f is a surjection from $\mathcal{V}$ onto $\mathrm{Image}(f)$.

On the other hand, suppose that $f(\vec{v}_1) = f(\vec{v}_2)$ for some $\vec{v}_1, \vec{v}_2$ in $\mathcal{V}$. Then $f(\vec{v}_1 - \vec{v}_2) = \vec{0}$, so $\vec{v}_1 - \vec{v}_2$ is in $\mathrm{Null}(f)$. But $\vec{v}_1 - \vec{v}_2$ is also in $\mathcal{V}$, which is a complement of $\mathrm{Null}(f)$; so $\vec{v}_1 - \vec{v}_2 = \vec{0}$; so $\vec{v}_1 = \vec{v}_2$. Thus f is an injection over $\mathcal{V}$. ∎.

Corollary 4.42. $\mathrm{Dim}(\mathrm{Image}(f)) + \mathrm{Dim}(\mathrm{Null}(f)) = n$.

Proof: Let $\mathcal{V}$ be the complement of $\mathrm{Null}(f)$. By theorems 4.41 and 4.39, $\mathrm{Dim}(\mathrm{Image}(f)) = \mathrm{Dim}(\mathcal{V})$ and by theorem 4.26 $\mathrm{Dim}(\mathrm{Null}(f)) + \mathrm{Dim}(\mathcal{V}) = n$. ∎

4.15 Inverses

Theorem 4.43. *If f is invertible, then f^{-1} is a linear transformation and $m = n$.*

Proof: Since f is linear we have $f(a \cdot f^{-1}(\vec{v})) = a \cdot f(f^{-1}(\vec{v})) = a\vec{v}$ and $f(f^{-1}(\vec{v}) + f^{-1}(\vec{u})) = f(f^{-1}(\vec{v})) + f(f^{-1}(\vec{u})) = \vec{v} + \vec{u}$. Applying f^{-1} to both sides of both equations we have $f^{-1}(a\vec{v}) = af^{-1}(\vec{v})$ and $f^{-1}(\vec{v} + \vec{u}) = f^{-1}(\vec{v}) + f^{-1}(\vec{u})$, so f^{-1} is a linear transformation.

By corollary 4.40 since f has a left inverse, we have $m \geq n$, and since f^{-1} has a left inverse, we have $n \geq m$, so $m = n$. ∎.

A matrix that has no full inverse is said to be *singular*. A matrix that has an inverse is said to be *non-singular*.

Theorem 4.44. *If f is a linear transformation and an injection from $\mathbb{R}^n$ to $\mathbb{R}^m$ then there exists a left inverse g that is a linear transformation.*

Proof: Let $\mathcal{V}$ be a complement for Image(f) in $\mathbb{R}^m$. Define the function $g(\vec{w})$ from $\mathbb{R}^m$ to $\mathbb{R}^n$ as follows

> Let $\vec{w} = \vec{u} + \vec{v}$ where $\vec{u}$ is in Image(f) and $\vec{v}$ is in $\mathcal{V}$; (this is unique, since these spaces are complements).
> Let $\vec{x}$ be the vector in $\mathbb{R}^n$ such that $f(\vec{x}) = \vec{u}$; (this exists since $\vec{u}$ is in Image(f) and is unique since f is an injection).
> Let $g(\vec{w}) = \vec{x}$.

It is easily shown that g is a left inverse for f and that g is a linear transformation. ∎

Corollary 4.45. *If matrix F is an injection, then F has an left inverse G, such that $G \cdot F = I_n$.*

Theorem 4.46. *If f is a linear transformation and an surjection from $\mathbb{R}^n$ to $\mathbb{R}^m$ then there exists a right inverse h that is a linear transformation.*

Proof: Let $\mathcal{V}$ be a complement for Null(f) in $\mathbb{R}^n$. By theorem 4.41, f is a bijection between $\mathcal{V}$ and $\mathbb{R}^m$, so for any $\vec{x}$ in $\mathbb{R}^m$ there exists a unique $\vec{v}$ in $\mathcal{V}$ such that $f(\vec{v}) = \vec{x}$. Define $h(\vec{x}) = \vec{v}$. It is easily shown that h is a right inverse and a linear transformation. ∎

Corollary 4.47. *If matrix F is an surjection, then F has an right inverse H, such that $F \cdot H = I_m$.*

4.16 Systems of linear equations

We are now able to characterize the space of solutions to systems of linear equations with a given matrix F of coefficients.

Theorem 4.48. *The system of linear equations $F \cdot \vec{x} = \vec{b}$ has a solution just if $\vec{b}$ is in* Image(f).

Proof: Immediate from the meaning of Image(f) and the correspondence between f and F. ∎

Theorem 4.49. *The system of linear equations $F \cdot \vec{x} = \vec{b}$ has a solution for every $\vec{b}$ if and only if* Rank(F) = m.

Proof: m = Rank(f) = Dim(Image(f)) if and only if Image(f) = $\mathbb{R}^m$. ∎

Definition 4.12. *Let F be an $m \times n$ matrix.*
The row space *of F is the span of its rows,* Span($F[1,:], F[2,:], \ldots F[m,:]$)*; this is a subspace of $\mathbb{R}^n$.*
The column space *of F is the span of its columns,* Span($F[:,1], F[:,2], \ldots F[:,n]$)*; this is a subspace of $\mathbb{R}^m$.*

Theorem 4.50. *The image of F is the span of its columns:* Image(F) = Span($F[:,1] \ldots F[:,n]$).

Proof: Immediate from the fact that $F \cdot \vec{v} = \vec{v}[1] \cdot F[:,1] + \ldots + \vec{v}[n] \cdot F[:,n]$

Theorem 4.51. Null(F) *is the orthogonal complement of the row space of F.*

Proof: Vector $\vec{v}$ is in Null(F) if and only if $F \cdot \vec{v} = \vec{0}$. But $F \cdot \vec{v} = \langle F[1,:] \cdot \vec{v}, \ldots, F[m,:] \cdot \vec{v}$, the vector consisting of the dot product of each row with $\vec{v}$, so this product is $\vec{0}$ only if $\vec{v}$ is orthogonal to each of the rows in F – that is, if $\vec{v}$ is in the orthogonal complement of the row space of F. ∎

Note that the previous two theorems come from the two different views of matrix multiplication mentioned in section 3.7.

Corollary 4.52. *Let R be the row space of matrix F. Then* $\text{Rank}(F) = \text{Dim}(\text{Image}(F)) = \text{Dim}(R) = n - \text{Dim}(\text{Null}(F))$.

Proof: By theorems 4.51 and 4.26 we have $\text{Dim}(R) + \text{Dim}(\text{Null}(F)) = n$. By corollary 4.42 we have $\text{Dim}(\text{Image}(F)) + \text{Dim}(\text{Null}(F)) = n$. ∎

Putting all this together, we can amplify the description of the categories of matrices given in part I.

Category I: $\text{Rank}(F) = m = n$. F is a non-singular square matrix. The rows of F and the columns of F are both bases for $\mathbb{R}^n$. F is a bijection from $\mathbb{R}^n$ to itself. $\text{Image}(F) = \mathbb{R}^n$. $\text{Null}(F)$ is the zero space. F has a full inverse. The system $F \cdot \vec{x} = \vec{b}$ has a unique solution for all $\vec{b}$.

Category II: $\text{Rank}(F) = m < n$. The rows of F are linearly independent but do not span $\mathbb{R}^n$. The columns of F span $\mathbb{R}^m$ but are linearly dependent. F is a surjection from $\mathbb{R}^n$ to $\mathbb{R}^m$ but not an injection. $\text{Image}(F) = \mathbb{R}^m$. $\text{Null}(F)$ is not the zero space. $\text{Dim}(\text{Null}(F)) = n - m$. F has a right inverse. The system $F \cdot \vec{x} = \vec{b}$ has infinitely many solutions for every $\vec{b}$. The system of equations is *underconstrained*.

Category III: $\text{Rank}(F) = n < m$. The columns of F are linearly independent but do not span $\mathbb{R}^m$. The rows of F span $\mathbb{R}^n$ but are linearly dependent. F is an injection from $\mathbb{R}^n$ to $\mathbb{R}^m$ but not an surjection. $\text{Image}(F) \neq \mathbb{R}^m$. $\text{Dim}(\text{Image}(F)) = n$. $\text{Null}(F)$ is the zero space. F has a left inverse. The system $F \cdot \vec{x} = \vec{b}$ does not have solutions for every $\vec{b}$; for any value of $\vec{b}$ it has at most one solution. The system of equations is *overconstrained*.

Category IV: $\text{Rank}(F) < m$, and $\text{Rank}(F) < n$. The rows and the columns are each linearly dependent; the rows do not span $\mathbb{R}^n$ and the columns do not span $\mathbb{R}^m$. F is neither an injection nor a surjection. $\text{Image}(F) \neq \mathbb{R}^m$. $\text{Dim}(\text{Image}(F)) < \min(m, n)$. $\text{Null}(F)$ is not the zero space. $\text{Dim}(\text{Null}(F)) > \max(n-m, 0)$. F has neither a left inverse nor a right inverse. The system $F \cdot \vec{x} = \vec{b}$ does not have solutions for every $\vec{b}$. If $F \cdot \vec{x} = \vec{b}$ has a solution for a particular value of $\vec{b}$ then it has infinitely many solutions for that value.

In principle, if we can compute a right inverse or a full inverse H for F, then we can solve the system of linear equations $F\vec{x} = \vec{b}$ as $H\vec{b}$ since $FH\vec{b} = \vec{b}$. If we can compute a left image G for F, and if the system $F\vec{x} = \vec{b}$ has a solution then, applying G to both sides of the equation we see that $\vec{x} = GF\vec{x} = G\vec{b}$. Note, however, that $G\vec{b}$ is not necessarily a solution to the equation since $FG\vec{b}$ is not necessarily equal to $\vec{b}$; all we can be sure of is that *if* a solution exists, then it must be equal to $G\vec{b}$. However, as we shall see in chapter 5 these are not in practice the best way to solve systems of linear equations, even aside from the fact that they do not apply to systems in category IV.

Part III: Vector spaces in general (Very optional)

4.17 The general definition of vector spaces

In this section we give a much more general definition of a vector space, which is standard in the mathematical literature, and we illustrate it with a few examples. Nothing in this section will be needed in the remainder of this book.

First we need to define a *field*. A field is a set on which we can define addition and multiplication operators that have some of the properties that we are used to in the real numbers.

Definition 4.13. *A* field *consists of a set of elements, one of which is named "0" and another of which is named "1", and two binary functions, named "+" and "∗", satisfying the following axioms.*

1. $0 \neq 1$.
2. *For all* a *and* b, $a + b = b + a$.
3. *For all* a, b, *and* c, $(a + b) + c = a + (b + c)$
4. *For all* a, $a + 0 = a$.
5. *For all* a *there exists an element* b *such that* $a + b = 0$.
6. *For all* a *and* b, $a * b = b * a$.
7. *For all* a, b, *and* c, $(a * b) * c = a * (b * c)$
8. *For all* a, $a * 1 = a$.
9. *For all* $a \neq 0$ *there exists an element* b *such that* $a * b = 1$.
10. *For all* a, b, *and* c, $(a + b) * c = (a * c) + (b * c)$.

The set of real numbers is a field. Other examples of fields include:

- The rational numbers.
- The complex numbers.
- For some fixed integer r, all numbers of the form $p + q\sqrt{r}$, where p and q are rational.
- For any prime p, the numbers $0 \ldots p - 1$, where $+$ and $*$ are interpreted as addition and multiplication modulo p. All the axioms except (9), the existence of a multiplicative inverse, are immediate; proving (9) takes a little more work.
- The set of all rational polynomials; that is, all fractions $f(x)/g(x)$ where $f(x)$ and $g(x)$ are polynomials and $g(x) \neq 0$.

We can now give the general definition of a vector space.

Definition 4.14. *Let* $\mathcal{F}$ *be a field; the elements of* $\mathcal{F}$ *are called* scalars. *A* vector space over $\mathcal{F}$ *consists of a collection of elements, called* vectors, *one of which is called "*$\vec{0}$*", and two operations. The first operation is named "+" and takes two vectors as arguments. The second operation is named "∗" and takes a scalar and a vector as arguments. The operations satisfy the following axioms:*

- *For any vectors* $\vec{u}$ *and* $\vec{v}$, $\vec{u} + \vec{v} = \vec{v} + \vec{u}$.
- *For any vectors* $\vec{u}$, $\vec{v}$, *and* $\vec{w}$, $(\vec{u} + \vec{v}) + \vec{w} = \vec{u} + (\vec{v} + \vec{w})$.
- *For any vector* $\vec{u}$, $\vec{u} + \vec{0} = \vec{u}$.
- *For any scalars* a, b *and vector* $\vec{v}$, $a * (b * \vec{v}) = (a * b) * \vec{v}$.
- *For any vector* $\vec{u}$, $0 * \vec{u} = \vec{0}$ *and* $1 * \vec{u} = \vec{u}$.
- *For any scalars* a, b *and vector* $\vec{v}$, $(a + b) * \vec{v} = (a * \vec{v}) + (b * \vec{v})$.
- *For any scalar* a *and vectors* $\vec{u}, \vec{v}$, $a * (\vec{u} + \vec{v}) = (a * \vec{u}) + (a * \vec{v})$.

A few examples of vector spaces (in each of these, the definition of vector sum and of scalar multiplication is the obvious one):

- For any field $\mathcal{F}$ and fixed n, define a vector to be an n-tuples of elements of $\mathcal{F}$.
- For any field $\mathcal{F}$ and any set S, define a vector to be a function from S to $\mathcal{F}$.
- Define a vector f to be a differentiable function from $\mathbb{R}$ to $\mathbb{R}$.
- Define a vector f to be a function from $\mathbb{R}$ to $\mathbb{R}$ such that the integral $\int_{-\infty}^{\infty} f^2(x)\,dx$ exists and is finite.

It should be emphasized that all the discussion of vectors and vectors spaces in this book, outside this single section, assumes that the vectors are in $\mathbb{R}^n$. Therefore, it is not safe to assume that the theorems in this book apply, or can be modified to apply, to any other kind of vectors; or that the definitions are correct or even meaningful. For example, for vectors over the complex numbers, the definition of the dot product has to be slightly changed. For continuous functions viewed as vectors, the definition of the dot product has to be substantially changed. For vectors over finite fields, the concept of a dot product is not useful.

Exercises

Exercise 4.1

Which of the following sets of vectors are vector spaces? Justify your answer in each case.

A. $\mathbb{R}^2 \cup \mathbb{R}^3$.

B. $\{\langle x, 2x\rangle \quad x \in \mathbb{R}\}$

C. $\{\langle k, 2k\rangle \mid k \text{ is an integer }\}$.

D. $\{\langle x, 2x + 1\rangle \mid x \in \mathbb{R}\}$.

E. $\{\langle x, 0\rangle \mid x \in \mathbb{R}\} \cup \{\langle 0, y\rangle \mid y \in \mathbb{R}\}$.

F. $\text{Span}(\{\langle 1, 3, 2\rangle, \langle -1, 0, 3\rangle\})$.

Exercise 4.2

For each of the following sets of three-dimensional vectors, state whether or not it is linearly independent. Justify your answers.

A. $\{\langle 1, 2, 3\rangle\}$

B. $\{\langle 1, 1, 0\rangle, \langle 0, 1, 1\rangle\}$

C. $\{\langle 1, 1, 0\rangle, \langle 2, 2, 1\rangle\}$.

D. $\{\langle 1, 1, 0\rangle, \langle 2, 2, 0\rangle\}$.

E. $\{\langle 2.3, 4.5, -1.2\rangle, \langle 3.7, 1.2, 4.3\rangle, \langle 0, 1.4, 2.5\rangle, \langle -2.9, -3.1, 1.8\rangle\}$ (Hint: It should not be necessary to do any calculations involving the components.)

Exercise 4.3

In the example illustrating theorem 4.5, page 76 verify that, as claimed

$|\vec{u}| = |\operatorname{Coords}(\vec{u}, \mathcal{N})| = \sqrt{74}$;
$|\vec{v}| = |\operatorname{Coords}(\vec{v}, \mathcal{N})| = \sqrt{146}$; and
$\vec{u} \bullet \vec{v} = \operatorname{Coords}(\vec{u}, \mathcal{N}) \bullet \operatorname{Coords}(\vec{v}, \mathcal{N}) = 69$.

Exercise 4.4

Let $\mathcal{U} = \operatorname{Span}(\{\langle 1, 0, 0, 0\rangle, \langle 0, 1, 0, 0\rangle\})$ and $\mathcal{V} = \operatorname{Span}(\{\langle 1, 1, 0, 0\rangle, \langle 0, 0, 1, 1\rangle\})$ be subspaces of $\mathbb{R}^4$.

A. Give a basis for $\mathcal{U} \oplus \mathcal{V}$.

B. Give a basis for $\mathcal{U} \cap \mathcal{V}$.

Exercise 4.5

(Do this by hand, in terms of square roots, if you can; if not, use MATLAB.)
Let $\mathcal{U} = \operatorname{Span}(\{\langle 1, 0, 1, 0\rangle, \langle 1, 1, 1, 1\rangle\})$ be a subspace of $\mathbb{R}^4$.

A. Find an orthonormal basis for $\mathcal{U}$.

B. Extend your answer in (A) to an orthonormal basis for $\mathbb{R}^4$.

Exercise 4.6

What is the dimension of the space spanned by the following four vectors? (Do this both by hand and using MATLAB.)

$$\langle 1, 2, 2, -1\rangle, \langle 0, 1, -1, 0\rangle, \langle 1, 4, 0, -1\rangle, \langle 2, 1, 1, -1\rangle.$$

Exercise 4.7

Let $\mathcal{V} = \text{Span}(\{\langle 1, 1, 0, 3\rangle; \langle 2, 4, -3, 1\rangle; \langle 7, 9, -6, 5\rangle\})$. Using MATLAB, determine whether the vector $\langle 1, 3, -4, 0\rangle$ is in $\mathcal{V}$.

Problems

Problem 4.1

Prove theorem 4.4. In this problem and in problems 4.2 and 4.3, though the statement of the theorem is in part I of the chapter, you should master the material in the corresponding section of part II before attempting this problem.

Problem 4.2

Prove theorem 4.7.

Problem 4.3

Prove theorem 4.8, parts a and b.

Problem 4.4

Prove theorem 4.36. (Hint: Consider example 4.6.)

Problem 4.5

(Use MATLAB. Since the answer is not at all unique, you should submit the code you used to compute it, not just the numeric answer.)

Let $\mathcal{U} = \text{Span}(\{\langle 1, 2, 3, 4, 3, 2, 1\rangle,\ \langle 4, 0, 2, 0, -2, 0, -4\rangle,\ \langle 3, 1, 2, 0, 1, -1, 0\rangle\})$ and
$\mathcal{V} = \text{Span}(\{\langle 2, 1, 3, 4, 0, 3, -3\rangle,\ \langle 4, 3, 5, 4, 4, 1, 1\rangle,\ \langle 1, 1, 1, 1, 1, 1, 2\rangle\})$ be subspaces of $\mathbb{R}^7$.

A. Find an orthogonal basis for $\mathcal{U} \cap \mathcal{V}$.

B. Extend your answer in (A) to an orthogonal basis for $\mathcal{U} \oplus \mathcal{V}$.

C. Check your answer.

Problem 4.6

As discussed in problem 3.6, an $n \times n$ matrix A is nilpotent if $A^p = 0$ for some power p. Prove that, if $A^p = 0$ and A has rank r then $p \cdot (n - r) \geq n$.

Programming Assignments

Assignment 4.1: Extracting a basis

Write a MATLAB function "FindBasis(A)" which does the following. The input A is an $m \times n$ matrix which we will view as m n-dimensional vectors. The value returned is a $p \times n$ matrix containing a subset (or all) of the rows of A that form a basis for the subspace spanned by the rows of A.

For instance if

$$A = \begin{bmatrix} 1 & 0 & 1 & 2 \\ 2 & 0 & 2 & 4 \\ 1 & -1 & 1 & 1 \end{bmatrix}$$

then FindBasis(A) should return either

$$\begin{bmatrix} 1 & 0 & 1 & 2 \\ 1 & -1 & 1 & 1 \end{bmatrix} \qquad \text{or} \qquad \begin{bmatrix} 2 & 0 & 2 & 4 \\ 1 & -1 & 1 & 1 \end{bmatrix}$$

If

$$A = \begin{bmatrix} 1 & 0 & 1 & 2 \\ 0 & 1 & 1 & 1 \\ 1 & -1 & 0 & 1 \end{bmatrix}$$

then FindBasis(A) should return a 2×4 matrix with any two of the rows of A.
If

$$A = \begin{bmatrix} 1 & 0 & 1 & 2 \\ 0 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \end{bmatrix}$$

then FindBasis(A) should return A.

Chapter 5

Algorithms

The theory developed in previous chapter is very elegant. Unfortunately, it presents almost no algorithms to compute actual answers to the questions raised. (The only algorithm there is Gram-Schmidt orthogonalization.)

In this chapter we present two algorithms. The first is *Gaussian elimination*, which reduces a matrix to *row-echelon form.* This will allow us to solve a system of linear equations, to compute the rank of a matrix, and to compute the coordinates of a given vector relative to a given basis. The second is the computation of the inverse of a matrix.

5.1 Gaussian elimination: Examples

We begin with two examples of solving systems of simultaneous equations using Gaussian elimination.

Example 5.1

Consider the following system of equations:

$$\begin{array}{llrcrcrcr} (1) & 2x & - & 4y & + & 2z & = & -8 \\ (2) & 2x & + & 2y & + & z & = & 5 \\ (3) & x & + & y & - & 2z & = & 5 \end{array}$$

Step 1.A: Subtract equation (1) from equation (2), giving $6y - z = 13$.

Step 2.B: Subtract 1/2 equation (1) from equation (3), giving $3y - 3z = 9$.

The system is now

$$\begin{array}{llrcrcrcr} (1) & 2x & - & 4y & + & 2z & = & -8 \\ (2) & & & 6y & - & z & = & 13 \\ (3) & & & 3y & - & 3z & = & 9 \end{array}$$

Step 3: Subtract 1/2 equation (2) from equation (3), giving $(-5/2)z = 5/2$.

The system is now

$$\begin{array}{llrcrcrcr} (1) & 2x & - & 4y & + & & 2z & = & -8 \\ (2) & & & 6y & - & & z & = & 13 \\ (3) & & & & & (-5/2)z & = & 5/2 \end{array}$$

The system is now easily solved. By equation (3) we have $z = -1$. Substituting this into equation 2, we get $y = 2$. Substituting these two values into equation (1), we get $x = 1$.

Example 5.2

More complex issues arise in the following system of 4 equations in 4 unknowns:

$$\begin{array}{llcrcrcrcr} (1) & w & + & x & + & y & + & z & = & 5 \\ (2) & w & + & x & + & 2y & + & 2z & = & 7 \\ (3) & & & x & - & y & + & z & = & -2 \\ (4) & w & & & + & 2y & & & = & 7 \end{array}$$

Step 1a: Subtract equation (1) from equation (2), giving $y + z = 2$.

Step 1b: Subtract equation (1) from equation (4), giving $-x + y - z = 2$. Multiply by -1 giving $x - y + z = -2$.

The system is now

$$\begin{array}{llcrcrcrcr} (1) & w & + & x & + & y & + & z & = & 5 \\ (2) & & & & & y & + & z & = & 2 \\ (3) & & & x & - & y & + & z & = & -2 \\ (4) & & & x & - & y & + & z & = & -2 \end{array}$$

Step 2: Switch equations 2 and 3 (just a reordering). The system is now

$$\begin{array}{llcrcrcrcr} (1) & w & + & x & + & y & + & z & = & 5 \\ (2) & & & x & - & y & + & z & = & -2 \\ (3) & & & & & y & + & z & = & 2 \\ (4) & & & x & - & y & + & z & = & -2 \end{array}$$

Step 3: Subtract equation (2) from equation (4). The system is now

$$\begin{array}{llcrcrcrcr} (1) & w & + & x & + & y & + & z & = & 5 \\ (2) & & & x & - & y & + & z & = & -2 \\ (3) & & & & & y & + & z & = & 2 \\ (4) & & & & & & & 0 & = & 0 \end{array}$$

This system is now easily solved. Starting with equation (3), we can assign z to be an arbitrary value, and y to be $2 - z$; we will choose $z = 0, y = 2$. By equation (2) $x = 0$. By equation (1), $w = 3$.

5.2 Gaussian elimination: Discussion

The procedure used to solve a system S of linear equations in the previous section is divided into two parts:

- Use the *Gaussian elimination algorithm* to convert the input system into an *equivalent* system R in *row echelon form*.
- Use a simple procedure to find the solutions to R.

We will now discuss each part of this description.

Definition 5.1. *Two systems of linear equations $S1$ and $S2$ are* equivalent *if they have the same solution space.*

Definition 5.2. *An n-dimensional vector $\vec{v}$ has k* leading zeros *if either*

- $\vec{v} = \vec{0}$ *and* $k = n$*; or*
- $\vec{v}[i] = 0$ *for* $i = 1 \ldots k$ *and* $\vec{v}[k+1] \neq 0$.

Definition 5.3. *Let A be an $m \times n$ matrix. A is in* row echelon form *if, for each row $A[i,:]$, either $A[i,:] = \vec{0}$ or $A[i,:]$ has more leading zeros than $A[i-1,:]$. A system of linear equations $A\vec{x} = \vec{c}$ is in row echelon form if A is in row echelon form.*

If the system of equations $A\vec{x} = \vec{c}$ is in row echelon form, then a solution can easily be found using the algorithm SolveRowEchelon shown in table 5.1.

```
function L(A, i)
    return the number of leading zeros in A[i, :].

    /* SolveRowEchelon(A, c) takes as arguments an m × n matrix A in row echelon form
    and an m-dimensional vector c. If the system of equations Ax = c has a solution, then
    the algorithm returns one such solution. If the system has no such solution, then the
    algorithm returns false */

procedure SolveRowEchelon(A, c)
    if (there exists i for which A[i, :] = 0 and c[i] ≠ 0)
      then return false; /* The ith equation is 0 · x[1] + ... + 0 · x[n] = c ≠ 0 */
      else if A = 0 then return any n-dimensional vector; /* the system is 0 · x = 0 */
      else let t be the largest value for which A[t, :] ≠ 0
      let x be an n-dimensional vector;
      for (i ← t downto 1)
          p ← L(A, i)+1;
          if (i = m) then q ← n else q ← L(A, i + 1);
          if (p < q)
            then for (q downto p + 1)
                    x[j] ← an arbitrary value;
                 endfor
          endif
          x[p] ← (c[i] − Σ_{j=p+1}^{n} A[i, j] · x[j])/A[i, p];
    endfor
    return x;
endif
end SolveRowEchelon
```

Table 5.1: Solving a system of equations in row-echelon form

It is easy to see that the value $\vec{x}$ returned by procedure SolveRowEchelon satisfies the system of equation. The procedure fills in values of $\vec{x}$ from bottom to top. At each iteration of the loop, the procedure deals with the ith equation. Because the system is in row-echelon form, the variable corresponding to the first non-zero coefficient is not yet set, and can be set in a way that satisfies the equation.

The Gaussian elimination procedure to convert a system of equations to row-echelon form is given in table 5.2:

```
    /* GaussianEliminate(A, c⃗) takes an m × n matrix A and an m-dimensional vector c⃗. It
    converts the system of equations Ax⃗ = c⃗ to an equivalent system in row-echelon form.
    */

procedure GaussianEliminate(A, c⃗)
for (i ← 1 to m) /* i is the row we are working on */
    if (A[p, :] = 0⃗ for all p ≥ i) then exitloop;
    j ← the smallest value such that A[p, j] ≠ 0 for some p ≥ i; /* j is the column we are working on. */
    q ← argmax_{p≥i} |A[p, j]|;
        /* q is the index of the row p ≥ i with the largest value (in absolute value) in the jth column. */
    if (q ≠ i) then { swap(A[i, :], A[q, :]);
                      swap(c⃗[i], c⃗[q]); }
    c⃗[i] ← c⃗[i]/A[i, j]; /* Divide equation i by A[i, j]. */
    A[i, :] ← A[i, :]/A[i, j];
    /* Subtract the appropriate multiple of the ith equation from each of the lower equations
       to zero out the jth column. */
    for (p ← i + 1 to m)
        c⃗[p] ← c⃗[p] − A[p, j] · c⃗[i];
        A[p, :] ← A[p, :] − A[p, j] · A[i, :];
    endfor
endfor
return A, c⃗
end GaussianEliminate
```

Table 5.2: Gaussian Elimination

It is easily seen that the following loop invariant holds after the ith iteration of the main loop of procedure GaussianEliminate: Let j be the index of the first non-zero component of $A[i, :]$ (that is, $j = \mathrm{L}(A, i)$). Then

- $A[i, j] = 1$
- For all $p > i$ and all $q \leq j$, $A[p, q] = 0$.

Thus, when the loop exits (either because $i = m$ or all the remaining rows are now $\vec{0}$) the matrix A will be in row-echelon form.

To show that the input and output sets of equations are equivalent, we note that the execution of the algorithm consists of a sequence of three different kinds of operations on the systems of equations:

i. Change the order of the equations.

ii. Multiply an equation by a non-zero scalar.

iii. For some p, i, replace the pair of equations
   (1) $A[i, :] \cdot \vec{x} = \vec{c}[i]$;
   (2) $A[p, :] \cdot \vec{x} = \vec{c}[p]$
   by the pair of equations
   (1) $A[i, :] \cdot \vec{x} = \vec{c}[i]$;
   (3) $(A[p, :] + \alpha \cdot A[i, :]) \cdot \vec{x} = \vec{c}[p] + \alpha \cdot \vec{c}[i]$.

It is trivial that operations (i) and (ii) do not change the solution space. To show that operation (iii) does not change the solution space, note that, if (1) and (2) are true for a particular $\vec{x}$, then (3) can be derived by multiplying (1) by α and adding it to (2); and if (1) and (3) are true, then (2) can be derived by multiplying (1) by $-\alpha$ and adding it to (3). Thus the two pairs of equations are equivalent.

We can now put the two procedures together into a method for solving systems of linear equations (table 5.3).

> /* SolveLinearEqns($A, \vec{c}$) takes as arguments an $m \times n$ matrix A and an m-dimensional vector $\vec{c}$. If the system has a solution, then it returns one solution; otherwise, it returns **false** */

procedure SolveLinearEqns($A, \vec{c}$)
return SolveRowEchelon(GaussianEliminate($A, \vec{c}$))

Table 5.3: Solving a System of Linear Equations

Based on our discussion above we can state a number of theorems:

Theorem 5.1. *Let A be an $m \times n$ matrix A and let $\vec{c}$ be an m-dimensional vector. Let $A', \vec{c}'$ be the values returned by GaussianEliminate($A, \vec{c}$). Then the system of equations $A'\vec{x} = \vec{c}'$ is in row-echelon form and is equivalent to the system $A\vec{x} = \vec{c}$.*

Theorem 5.2. *Let A be an $m \times n$ matrix in row-echelon form and let $\vec{c}$ be an m-dimensional vector. If the system of equations $A\vec{x} = \vec{c}$ has a solution, then SolveRowEchelon($A, \vec{c}$) returns some solution to the system. If the system has no solution, then SolveRowEchelon($A, \vec{c}$) returns* **false**.

Theorem 5.3. *Let $A\vec{x} = \vec{c}$ be a system of linear equations. If this system has a solution, then SolveLinearEqns($A, \vec{c}$) returns a solution. If it does not, then SolveLinearEqns($A, \vec{c}$) returns* **false**

The procedure SolveLinearEqns can also be used to determine whether a vector $\vec{c}$ is in the vector space spanned by a given collection of vectors $\mathcal{B}$ and to find the coordinates of $\vec{c}$ in $\mathcal{B}$.

Theorem 5.4. *Let $\mathcal{B} = \{\vec{b}_1 \ldots \vec{b}_k\}$ be a set of vectors and let $\vec{c}$ be a vector. Let B be the matrix whose columns are $\vec{b}_1 \ldots \vec{b}_k$. Then $\vec{c}$ is in Span($\mathcal{B}$) if and only if the system $B\vec{x} = \vec{c}$ has a solution; if it does then any solution $\vec{x}$ is a coordinate vector for $\vec{c}$ in $\mathcal{B}$.*

Proof: Immediate from the fact that $B\vec{x}$ is the weighted sum of the columns of B:
$B\vec{x} = \vec{x}[1]B[:,1] + \ldots + \vec{x}[n]B[:,n]$. ∎

5.2.1 Gaussian elimination on matrices

The Gaussian elimination procedure can also be used to reduce a matrix A (rather than a system of equations) to row-echelon form; one can either delete the references to the constant vector $\vec{c}$ in the algorithm given in table 5.2 or, more simply, pass an arbitrary value for $\vec{c}$ and ignore the value returned. For this purpose, we will treat the procedure "GaussianEliminate(A)" as a function of one argument returning one value.

The following theorems then follow directly.

Theorem 5.5. *Let A be an $m \times n$ matrix, and let A' =GaussianEliminate(A). Then A' is in row-echelon form and the row span of A' is equal to the row span of A.*

Proof: The proof is exactly analogous to the proof of theorem 5.1. In particular, the proof that A' has the same row span as A works in exactly the same way as the proof that the system $A'\vec{x} = \vec{c}'$ is equivalent to the system $A\vec{x} = \vec{c}$.

Theorem 5.6. *If matrix A is in row-echelon form, then the non-zero rows of A are linearly independent.*

Proof: Let $A[i,:]$ be a non-zero row, and let $q = \mathrm{L}(A,i)+1$ be the position of the first non-zero value in $A[i,:]$, Since $A[i,q] = 1$ and $A[p,q] = 0$ for all $q > i$, clearly $A[i,:]$ is not a linear sum of the vectors $A[i+1,:] \ldots A[m,:]$. Applying corollary 4.15 to the non-zero rows in backward order, it follows that the rows are linearly independent.

Corollary 5.7. *Let A be any matrix. Then the non-zero rows of GaussianEliminate(A) are a basis for the row span of A, and Rank(A) is equal to the number of non-zero rows of GaussianEliminate(A).*

Proof: Immediate from theorems 5.5 and 5.6, together with the definitions of "basis" and "rank". ∎

5.2.2 Maximum element row interchange

There is one aspect of the Gaussian elimination algorithm that we have not yet explained. The second step of the main **for** loop finds the row q that maximizes $|A[q,i]|$, and the third steps swaps that with the ith row. Now, it is clear that to achieve row echelon form, if $A[i,i] = 0$, then we have to swap it with some row q where $A[q,i] \neq 0$. But why particularly the row with the largest absolute value?

In fact, if computers could do exact real-valued arithmetic — which, by the way, is the idealization used in all the above theorems — then it wouldn't matter which row we chose; any row q where $A[q,i] \neq 0$ would work just as well. But computers do not (normally) do exact real computation; they do floating point arithmetic, which is subject to round-off error. The point of the "maximum element row interchange" operation is that it reduces the error due to round-off. We will discuss the general issue of round-off a little further in section 5.6; for a detailed discussion of the maximum element row interchange rule, see (Trefethen and Bau, 1997).

5.2.3 Testing on zero

In a number of places in the above algorithms, there is a test whether a value is equal to zero. For instance, in SolveRowEchelon there is the instruction "**if** (there exists i for which $A[i,:] = \vec{0}$ and $\vec{c}[i] \neq 0$)"; in GaussianEliminate, there is "**if** ($A[p,:] = \vec{0}$ for all $p \geq i$) **then exitloop**;" and in the subroutine L there is, "return the number of leading zeros." Some of my friends who are numerical analysts object very strongly to these, saying that in actual computation you never test on zero, because in actual computation you never get zeros because of round-off errors and noise. (Some programming languages do not allow testing for equality between floating point numbers, for that reason.) By the same token theorems 5.1–5.7 are meaningless; they refer to conditions that are never met. You should simply carry out the computations without testing on zero; if you divide by zero at some stage, you will get `Inf` or `NaN`, but that is OK in MATLAB or any other system that meets the IEEE floating point standard (Overton 2001). When you have computed the final answer, then you evaluate it; if it contains either a very large value or `Inf` or `NaN`, then it may well not be meaningful.

The following experiment illustrates the difficulty in obtaining true zero with floating point arithmetic. Generate a random $n \times n-1$ matrix A and a random $n-1$ dimensional random column

vector $\vec{v}$. Set the nth column of A to be $A \cdot \vec{v}$. Now you have a random matrix[1] of rank $n-1$. Use the built-in MATLAB function `lu` to reduce A to row-echelon form, and test whether the last row is actually equal to the zero vector. Table 5.4 shows the success rate of this test, for each value of n. By contrast, the MATLAB function `rank(A)`, which uses a non-zero threshhold, always got the right answer of $n-1$ in all the experiments I ran, including 50×50 and 100×100 matrices.

n	2	3	4	5	6	10	20
Success rate	59%	15%	7.6%	5.2%	3.7%	1.9%	0.48%

Table 5.4: Frequency with which row-echelon reduction of a random singular matrix produces a final row equal to zero

Nonetheless, I have left these tests in for two reasons:

A. They don't do any harm. If they do not succeed then one has not lost anything by carrying them out. The only case where they arguably give a wrong result is in the case where the true value is very small, but due to round-off is computed as 0. In this case, including the test causes the algorithm to report that the matrix is singular, whereas if the test is eliminated, the algorithm returns an answer with some values being Inf or NaN. But this case is *extremely* rare, and the added value given by this answer is quite small.

B. As we will discuss in section 5.6, viewing these algorithms in terms of what can actually be accomplished with floating point operations is only one of several viewpoints one might take. If one considers the algorithm from the standpoint of pure mathematics or exact computation, then these tests and theorems 5.1-5.7 are valid.

5.3 Computing a matrix inverse

We now turn to the problem of inverting an $n \times n$ non-singular matrix. (We omit the problem of finding a left or right inverse of a non-square matrix; the techniques are analogous.)

The algorithm for computing the inverse modifies the Gaussian elimination algorithm in two ways. First, we continue carrying out the row transformation operations to reduce the matrix row-echelon form to the identity. Second, at the same time that we are carrying out operations to reduce the input matrix A to the identity, we carry out the same operations on a matrix C that starts as the identity. When we have carried out enough operations to reduce A to the identity, then the final state of C is A^{-1}.

The explanation of the modified version of the Gaussian elimination algorithm involves a few steps. First, we observe that, if R is in row-echelon form, we can reduce it to the identity by repeatedly subtracting $R_{i,j} \cdot R[j,:]$ from $R[i,:]$ for all $j > i$. Since $R[j,j] = 1$ for all j, this operation sets $R[i,j]$ to be 0. When we are done with all these, we will have

- For $i > j$, $R[i,j]$ was set to 0 in the initial translation of A to the row-echelon form R.
- For $i = j$, $R[i,j]$ was set to 1 in the initial translation of A to the row-echelon form R.
- For $i < j$, $R[i,j]$ has been set to 0 on this second pass of operations.

[1] There are other ways of generating random singular matrices which will give different distributions. There is no unique, obviously proper, notion of a "random singular matrix".

So R is now the identity (see example below).

Second, we observe that each of the operations that procedure GaussianEliminate(A) carries out corresponds to multiplication on the left by a specific matrix. Specifically:

1. Switching rows p and q of matrix A corresponds to forming the product $S^{p,q}A$, where $S^{p,q}$ is the matrix defined by
$$S^{p,q}[i,j] = \begin{cases} 1 & \text{if } i = j, i \neq p, i \neq q \\ 1 & \text{if } i = p, j = q \\ 1 & \text{if } i = q, j = p \\ 0 & \text{otherwise.} \end{cases}$$
For example, with $n = 5$, $p = 1, q = 4$ we have
$$S^{1,4} = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

2. Multiplying row p by α corresponds to forming the product $T^{p,\alpha}A$ where $T^{p,\alpha}$ is the matrix defined by
$$T^{p,\alpha}[i,j] = \begin{cases} 1 & \text{if } i = j, i \neq p \\ \alpha & \text{if } i = j = p \\ 0 & \text{otherwise.} \end{cases}$$
For example, with $p = 2, \alpha = 3.7$, we have
$$T^{2,3.7} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 3.7 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

3. Adding α times row p to row q corresponds to forming the product $P^{p,q,\alpha}A$ where $P^{p,q,\alpha}$ is the matrix defined by
$$P^{p,q,\alpha}[i,j] = \begin{cases} 1 & \text{if } i = j \\ \alpha & \text{if } i = q, j = p \\ 0 & \text{otherwise.} \end{cases}$$
For example, with $p = 2, q = 5, \alpha = -4.6$, we have
$$P^{2,5,4.6} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & -4.6 & 0 & 0 & 1 \end{bmatrix}$$

Therefore, the sequence of operations used to transform matrix A into its row echelon form R and to transform R into I corresponds to a sequence of matrix multiplications $R = M_t \cdot M_{t-1} \ldots M_2 \cdot M_1 A$ where M_1 is the matrix corresponding to the first operation performed by the Gaussian elimination algorithm, M_2 is the second operation, and so on. Therefore if we form the product $C = M_t \cdot M_{t-1} \ldots M_2 \cdot M_1$ then that is a matrix such that $CA = I$.

But (third) actually we don't have to generate these transformation matrices at all. Since $C = C \cdot I = M_t \cdot M_{t-1} \ldots M_2 \cdot M_1 \cdot I$ where I is the identity, we can get the effect of all these matrix multiplication just by initializing matrix C to be the identity, and then performing the same sequence of operations on C that we are performing on A. Thus we are implicitly computing the above matrix product. The resultant modified algorithm is shown in table 5.5.

(This argument may seem strange; we first replace the operations by the matrices S, T, and P, and then go back and replace the matrices by the same operations that we started with. What is the point of that? The point is we need to show that what the sequence of operations in the algorithm does *overall* in converting matrix A to row echelon form R consists of multiplying A on the left by a matrix C. To do this, we show that each operation corresponds to multiplication by a matrix, and therefore the sequence of operations, whether applied to A or applied to I^n, correspond to multiplication by the product of these. What the matrices corresponding to the individual operations actually *are* ends up not mattering.)

The algorithm for computing the inverse is given below. Note that if in the course of the initial conversion to row-echelon form, the leading zeros in one row increase from the previous row by more than 1, then the algorithm can immediately return with **fail**, signalling that the matrix is singular.

```
    /* Inverse(A) takes an n × n matrix A and returns A^{-1}. */

procedure Inverse(A)
B = A; C = I^n; /* Initialize C to be the identity.
                   At each stage of the algorithm, CB = A.
for (i ← 1 to n)
    q ← argmax_{p≥i} |B[q, i]|;
      /* q is the index of the row p from i with the largest value (in absolute value) in the ith column. */
    if B[q, i] = 0 then return fail; /* A is singular */
    if (q ≠ i) then { swap(B[i, :], B[q, :]);
                      swap(C[i, :], C[q, :]); }
    C[i, :] ← C[i, :]/B[i, i]; /* Divide row i in both matrices by B[i, i]. */
    B[i, :] ← B[i, :]/B[i, i];
    /* In both matrices, subtract the appropriate multiple of the ith row
    from each of the lower rows to zero out the ith column of B. */
    for (j ← i + 1 to n)
        C[j, :] ← C[j, :] − B[j, i] · C[i, :];
        B[j, :] ← B[j, :] − B[j, i] · B[i, :];
    endfor
endfor
    /* In both matrices, subtract the appropriate multiple of the ith row
    from each of the upper rows to zero out the ith column of B. */
for (i ← 2 to n)
    for (j ← 1 to n − 1)
        C[j, :] ← C[j, :] − B[j, i] · C[i, :];
        B[j, :] ← B[j, :] − B[j, i] · B[i, :];
    endfor
endfor
return C;
end Inverse.
```

Table 5.5: Computing Matrix Inverse

Example 5.3

We illustrate the above algorithm by computing the inverse of the matrix

$$A = \begin{bmatrix} 2 & 0 & 1 \\ -1 & 1 & 1 \\ 0 & 1 & 2 \end{bmatrix}$$

We first convert to row-echelon form.

$$B = \begin{bmatrix} 2 & 0 & 1 \\ -1 & 1 & 1 \\ 0 & 1 & 2 \end{bmatrix} \qquad\qquad C = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$B[1,:] = 1/2 * B[1,:]. \qquad C[1,:] = 1/2 * C[1,:]$$

$$B = \begin{bmatrix} 1 & 0 & 1/2 \\ -1 & 1 & 1 \\ 0 & 1 & 2 \end{bmatrix} \qquad C = \begin{bmatrix} 1/2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$B[2,:] = B[2,:] + B[1,:]. \qquad C[2,:] = C[2,:] + C[1,:]$$

$$B = \begin{bmatrix} 1 & 0 & 1/2 \\ 0 & 1 & 3/2 \\ 0 & 1 & 2 \end{bmatrix} \qquad C = \begin{bmatrix} 1/2 & 0 & 0 \\ 1/2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$B[3,:] = B[3,:] - B[2,:]. \qquad C[3,:] = C[3,:] - C[2,:]$$

$$B = \begin{bmatrix} 1 & 0 & 1/2 \\ 0 & 1 & 3/2 \\ 0 & 0 & 1/2 \end{bmatrix} \qquad C = \begin{bmatrix} 1/2 & 0 & 0 \\ 1/2 & 1 & 0 \\ -1/2 & -1 & 1 \end{bmatrix}$$

$$B[3,:] = B[3,:] * 2. \qquad C[3,:] = C[3,:] * 2$$

$$B = \begin{bmatrix} 1 & 0 & 1/2 \\ 0 & 1 & 3/2 \\ 0 & 0 & 1 \end{bmatrix} \qquad C = \begin{bmatrix} 1/2 & 0 & 0 \\ 1/2 & 1 & 0 \\ -1 & -2 & 2 \end{bmatrix}$$

We now continue on, converting B to the identity. We omit the steps where the factor is 0.

$$B[1,:] = B[1,:] - (1/2)B[3,:]. \qquad C[1,:] = C[1,:] - (1/2)C[3,:]$$

$$B = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 3/2 \\ 0 & 0 & 1 \end{bmatrix} \qquad C = \begin{bmatrix} 1 & 1 & -1 \\ 1/2 & 1 & 0 \\ -1 & -2 & 2 \end{bmatrix}$$

$$B[2,:] = B[2,:] - (3/2)B[3,:]. \qquad C[2,:] = C[2,:] - (3/2)C[3,:]$$

$$B = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad C = \begin{bmatrix} 1 & 1 & -1 \\ 2 & 4 & -3 \\ -1 & -2 & 2 \end{bmatrix}$$

We can now return

$$A^{-1} = C = \begin{bmatrix} 1 & 1 & -1 \\ 2 & 4 & -3 \\ -1 & -2 & 2 \end{bmatrix}$$

5.4 Inverse and systems of equations in MATLAB

The MATLAB utility for computing the inverse of matrix M could not be much simpler; just write `inv(M)` or `M^-1`. The MATLAB utility for computing the solution to the equations $M\vec{x} = \vec{c}$ could not be any simpler; just write `M\C`. (Note that $\vec{c}$ here must be a *column* vector). Of course, any half-decent programming environment provides a library function for solving systems of linear equations;[2] but it is not every language in which it is a single character.

The value returned by `M\C` depends on the characteristics of the system of equations. Let M be an $m \times n$ matrix.

Case 1. If $m = n = \text{Rank}(M)$ (i.e. M is a non-singular square matrix) then `M\C` returns the unique solution to the system of equations $M\vec{X} = \vec{C}$.

Case 2. If $m < n$ and $\text{Rank}(M) = m$, then `M\C` returns a solution to the equation $M\vec{X} = \vec{C}$ with the maximal number of zeros.

Case 3. If $m > n$ and $\text{Rank}(M) = n$, and the system $M\vec{X} = \vec{C}$ has a solution, then `M\C` returns that solution.

Case 4. If $m > n$ and $\text{Rank}(M) = n$, and the system $M\vec{X} = \vec{C}$ does not have a solution, then `M\C` returns the *least squares* best fit to the equations; that is, it returns the value of $\vec{X}$ such that $|M \cdot \vec{X} - \vec{C}|$ is minimal. This is discussed further in section 14.5.

For example, if

$$M = \begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 1 & 2 \end{bmatrix} \text{ and } C = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

then in MATLAB `X=M\C` returns

$$X = \begin{bmatrix} 0.3636 \\ 0.3636 \end{bmatrix}$$

Then `norm(M*X-C)` has the value 0.3015; this is smaller for this value of `X` than for any other value.

Case 5. If $\text{Rank}(M) < \min(m, n)$ and the system has no solution, then MATLAB will issue a warning and return an answer full of `NaN`'s and `Inf`'s.

Case 6. If $\text{Rank}(M) < \min(m, n)$ and the system has a solution then the result of `M\C` is hard to predict. It may return an answer with the warning "Rank deficient matrix", or it may return an answer full of `NaN`'s and `Inf`'s with the warning "Matrix is singular."

Examples of each of these are shown below.

You may wonder why underdetermined systems of equations are treated differently in case 2 and case 6. As the examples below demonstrate, if you give MATLAB the equation "$x + y = 2$" it happily returns the answer $x = 2, y = 0$; but if you give it the system of equations

$$\begin{array}{ccccc} x & + & y & = & 2 \\ x & + & y & = & 2 \end{array}$$

it huffily tells you that the matrix is singular, and gives the answer $x =$ `NaN`$, y =$ `NaN`. The reason for this difference is that the single equation is *well-conditioned* — a small change in the constant or

[2] Not all libraries have a very *good* function.

coefficients gives a correspondingly small change in the answer; whereas the system of two equations is *ill-conditioned* — a small change in the coefficients or constant may make the solution drastically different, or may even make the system inconsistent. This will be further discussed in section 5.5.

The MATLAB function `lu(M)` returns a pair of matrices $[L, U]$. U is the row-echelon reduction of M. L is the matrix corresponding to the product of the operations used in reducing M to U; thus $L \cdot U = M$. The pair $[L, U]$ is known as the LU factorization of M.

Examples:

```
% Example 5.1 above.

>> m=[2,0,1; -1,1,1; 0,1,2]

>> m
m =
     2     0     1
    -1     1     1
     0     1     2

>> inv(m)
ans =
     1     1    -1
     2     4    -3
    -1    -2     2

>> m^-1
ans =
     1     1    -1
     2     4    -3
    -1    -2     2

>> c=[2;5;7]
c =
     2
     5
     7

>> m\c
ans =
     0
     3
     2


% Cases of m\c:

% Case 1: Square, non-singular. m=n=Rank(M)

>> [1,2;2,1]\[4;5]
ans =
     2
     1
```

```
% Case 2: m=Rank(M) < n.

>> [1,1,1]\[3]
ans =
     3
     0
     0
>> [1,1,1;1,2,3]\[3;6]
ans =
    1.5000
         0
    1.5000

% Case 3: Rank(M)=n < m: System has a solution.

>> [1,1;2,1;1,2]\[2;3;3]
ans =
    1.0000
    1.0000

% Case 4: Rank(M)=n < m: System has no solution, so the best least squares
%         fit is returned.

>> [1,1;2,1;1,2]\[1;1;1]
ans =
    0.3636
    0.3636

>> [1,1;1,1;2,1]\[1;2;2]
ans =
    0.5000
    1.0000

% Case 5: Rank(M) < min(m,n), and no solution exists.
% {\sc Matlab} gives a warning and returns an answer full of NaN's and Inf's

>> [1,1;1,1]\[1;2]
Warning: Matrix is singular to working precision.
ans =
  -Inf
   Inf

% Case 6: Rank(M) < min(m,n), and a solution exists.
% {\sc Matlab} will certainly give a warning; it may or may not find a solution.


>> [1,1;1,1]\[2;2]
Warning: Matrix is singular to working precision.
ans =
   NaN
```

```
   NaN

>> [1,1,1;1,1,1]\[1;1]
Warning: Rank deficient, rank = 1,  tol =    9.4206e-16.
ans =
    1.0000
         0
         0



% LU decomposition, The examples are the coefficient matrices from
% the systems at the start of the chapter. Note that in both cases the
% value of U is the row-echelon decomposition that we computed above.

>> a=[2,-4,2;2,2,1;1,1,-2]
a =
     2    -4     2
     2     2     1
     1     1    -2

>> [l,u]=lu(a)
l =
    1.0000         0         0
    1.0000    1.0000         0
    0.5000    0.5000    1.0000
u =
    2.0000   -4.0000    2.0000
         0    6.0000   -1.0000
         0         0   -2.5000

>> l*u
ans =
     2    -4     2
     2     2     1
     1     1    -2

>> b=[1,1,1,1;1,1,2,2;0,1,-1,1;1,0,2,0]
b =
     1     1     1     1
     1     1     2     2
     0     1    -1     1
     1     0     2     0

>> [l,u] = lu(b)
l =
     1     0     0     0
     1     0     1     0
     0     1     0     0
     1    -1     0     1
u =
```

```
     1     1     1     1
     0     1    -1     1
     0     0     1     1
     0     0     0     0

>> l*u
ans =
     1     1     1     1
     1     1     2     2
     0     1    -1     1
     1     0     2     0
```

5.5 Ill-conditioned matrices

The Gaussian elimination algorithm described above, though unpleasant to work through by hand for any but very small systems, is easily understood, easily programmed, and generally quite effective and efficient. It is one of the most frequently executed algorithms on computers. (The algorithm for computing the inverse is substantially less important in practice.) It has been known in Western mathematics since Gauss published it in 1809 and in Chinese mathematics since about 200 AD or earlier. However, in rare cases, it gets into serious trouble.

We will not go at all deeply into this theory, but let us illustrate the problem with a (contrived) example. Consider the following system of equations:

$$\begin{array}{llcll} (1) & (1+10^{-9})x & + & y & = & 1 \\ (2) & x & + & (1-10^{-9})y & = & 1 \end{array}$$

It is easily verified that the solution is $x = 10^9, y = -10^9$. Now let us give this to MATLAB:

```
>> format long
>> d=10^-9
d =
   1.0000e-09
>> a=[1+d, 1; 1, 1-d]
a =
   1.000000001000000   1.000000000000000
   1.000000000000000   0.999999999000000
>> a\[1;1]
Warning: Matrix is close to singular or badly scaled.
         Results may be inaccurate. RCOND = 2.775558e-17.
ans =
   1.0e+06 *
  -9.007198990992798
   9.007199999999997
>>% Note that, as warned, the answer is nowhere near right.
```

Why is MATLAB freaking out here? The answer appears when we apply Gaussian elimination. Reducing the system to row echelon form involves two steps:

Let $d = 10^{-9}$

Step 1: Divide equation 1 by $1+d$ giving

$$\begin{array}{llllll} (3) & x & + & \frac{1}{1+d}y & = & \frac{1}{1+d} \\ (2) & x & + & (1-d)y & = & 1 \end{array}$$

Step 2: Subtract equation (3) from equation (2) giving

$$\begin{array}{llllll} (3) & x & + & \frac{1}{1+d}y & = & \frac{1}{1+d} \\ (4) & & & (1-d-\frac{1}{1+d})y & = & 1-\frac{1}{1+d} \end{array}$$

Now, note that $1-d = 0.999999999$ (exactly) but that

$$\frac{1}{1+d} = 1-d+d^2+d^3-\ldots = 0.9999999999000000000999...$$

. Therefore if you compute the coefficient of y in the above equation in the natural way, by first computing the fraction $\frac{1}{1+d}$ and then subtracting this from $1-d$, the calculation must be carried to 18 digits = 60 bits of precision, in order to detect that the coefficient is not actually 0. This is more than MATLAB ordinarily uses.

Another, related, problem is that the solution of the system of equations is extremely sensitive to the exact value of the constant terms (and equally sensitive to the exact values of the coefficients, though we will not illustrate that.) Suppose that the constant term in the first equation is changed by 1 part in a billion, from 1 to $1+10^{-9}$. Then the solution is obviously $x = 1, y = 0$. So changing one constant term from 1 to 1.000000001 changes the answer by 1,000,000,000!

In larger matrices, this sensitivity can turn up even with quite innocuous looking coefficients,

```
>> m=[1:7,9; 2:8,10; 3:8,10:11; 4:8,10:12; 5:8,10:13; 6:8,10:14; 7:8,10:15 ...
      8,10:16]

m =
     1     2     3     4     5     6     7     9
     2     3     4     5     6     7     8    10
     3     4     5     6     7     8    10    11
     4     5     6     7     8    10    11    12
     5     6     7     8    10    11    12    13
     6     7     8    10    11    12    13    14
     7     8    10    11    12    13    14    15
     8    10    11    12    13    14    15    16
>> b=1+(m/1000)
b =
    1.001  1.002  1.003  1.004  1.005  1.006  1.007  1.009
    1.002  1.003  1.004  1.005  1.006  1.007  1.008  1.010
    1.003  1.004  1.005  1.006  1.007  1.008  1.010  1.011
    1.004  1.005  1.006  1.007  1.008  1.010  1.011  1.012
    1.005  1.006  1.007  1.008  1.010  1.011  1.012  1.013
    1.006  1.007  1.008  1.010  1.011  1.012  1.013  1.014
    1.007  1.008  1.010  1.011  1.012  1.013  1.014  1.015
    1.008  1.010  1.011  1.012  1.013  1.014  1.015  1.016
>> (b\[1;1;1;1;1;1;1;1])'
ans =
 -125.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 125.0000
```

```
>> % Now we change one constant by 1 part in 1000 and ask the same question.
>> (b\[0.999;1;1;1;1;1;1;1])'

ans =
    4.6250 -1.0000 -1.0000 -1.0000 -1.0000 -1.0000 -1.0000 2.3750
```

Changing the first constant term from 1 to 0.999 changes the last component of the solution from 125 to 2.375. (One can get more extreme results than this, with the same matrix, but different constant vectors. See chapter 7, exercise 7.1.b).

Systems of equations of this kind, where the answers are extremely sensitive to the exact values of the constant terms and the coefficients, and therefore calculations must be carried out to extreme precision, are said to be *ill-conditioned.* In principle, ill-conditioned systems of equations should be rare; if you construct a system of equations constructed by choosing coefficients at random, then the probability it will be ill-conditioned is very small. Unfortunately among problems that actually arise in practice, ill-conditioned problems are quite common.

Dealing with ill-conditioned systems of equations raises two different kinds of issues. The first is an algorithmic problem; it is important to structure an algorithm so as to avoid the build-up of round-off error. Ill-conditioning greatly magnifies the inaccuracy due to round-off error; in dealing with ill-conditioned matrices, it is therefore especially important to use *numerically stable* algorithms which hold the round-off error to a minimum. This is the reason that the "maximum element row interchange rule" in row-echelon reduction is important (section 5.2.2).

The second issue is a modelling problem. Suppose that you are trying to solve a problem, and you formulate it as a system of linear equations, and it turns out that you get equations (1) and (2) above. Then unless you are quite sure that the equations, the coefficients, and the constant terms are all accurate to within a factor of better than one part in a billion, you may as well throw the equations in the garbage. Even if you carry out the computation exactly and get an answer of $x = 10^9, y = -10^9$, you have no reason to suppose that the true values are not $x = 1, y = 0$.

There is, of course, no algorithmic fix to the latter problem; there is no way to get answers that are fundamentally better than your data. Nonetheless, it is important to know when you are dealing with a ill-conditioned problem:

- You will know not to trust your answer.
- It is probably a good idea to look for some alternative way to formulate your problem.

We will discuss this issue further in section 7.7. For an extensive discussion see Trefethen and Bau, *Numerical Linear Algebra.*

5.6 Computational complexity

We conclude the chapter with a brief discussion of the computational complexity of the algorithms and problems discussed.[3] At the outset, there is a conceptual issue to address. There are actually three different ways to conceptualize numerical computations, such as solving systems of linear equations, each with its own drawbacks.

[3]In this section, we assume familiarity with the basic concepts of algorithmic analysis.

	Pure math	Exact computation	Floating point
Realizable	×	√	√
Exact answers	√	√	×
Reasonable computation time	√	×	√

Table 5.6: Viewpoints on numerical computation

In the first viewpoint, that of pure mathematics, the computation is idealized as exact arithmetic over real numbers. This is, in fact, the view taken in virtually this entire book, and it is the usual starting point, though not the ending point, for any discussion of numerical algorithms. (If an algorithm doesn't make sense in this idealized view, it is unlikely to make sense in any other view.) Computation time is viewed as the number of arithmetic operations plus the number of other algorithmic operations, but most computations of this kind are in any case dominated by the arithmetic operations. Theorems 5.1–5.7 are all true in this viewpoint, and the running times discussed below are all valid. The problem with this viewpoint is that the machine it runs on is imaginary; no actual computer can carry out arithmetic on real values to arbitrary precision in unit time per operation.

The second viewpoint, that of computation theory, is that the computation uses exact arithmetic over a class of numbers which is exactly representable in a finite data structure. For solving linear equations, the natural class of numbers would be the rational numbers; given any problem posed in terms of rational numbers, the exact answer and all the intermediate values calculated are also rational numbers. For more complex problems, such as those involving distance, it would be necessary to use an exact representation of algebraic numbers. Theorems 5.1–5.7 are valid in this viewpoint as well. Computation time is viewed in terms of bit operations; the time to add two integers is linear in the number of bits, and the time to multiply two integers is slightly more than linear.

However, for algorithms like Gaussian elimination, exact arithmetic on rational numbers is entirely impractical, because the number of bits required to maintain exactness increases exponentially with the size of the matrix. The time and space requirements therefore likewise increase exponentially. There are more sophisticated algorithms known that are polynomial in the number of bits (Yap 2000) but these involve complex techniques in algorithmic design and analysis, and are in any case impractical and not used. The computation time requirements given below are *not* valid on this viewpoint.

The third viewpoint is that of numerical analysis. Here the computation is viewed as involving floating point operation using some particular precision. Computation time is given in terms of number of machine instructions; one floating point operation is one machine instruction. This is, in fact, what is *always* actually done in useful numerical programs. The time requirements given below are valid in this viewpoint.

However, floating point operations inevitably involve round-off error, so theorems 5.1–5.7 are no longer exactly true. Indeed, the whole standard notion of program correctness — that the answer obtained is always the exact answer to the question — goes out the window in this viewpoint. It is replaced by the notion of *numerical stability*. A floating point algorithm $A(x)$ is a numerically stable algorithm for the mathematical function $f(x)$ if for every x, there exists some $\bar{x}$ such that $\bar{x}$ is close to x (as compared to the precision of the floating point system) and $A(\bar{x})$ is close to $f(\bar{x})$. In an implementation with round-off, this is the best that one can hope for. The Gaussian elimination algorithm given above is numerically stable in all but a small number of pathological cases; with further improvements, it can be made numerically stable in all cases.

Table 5.6 summarizes these pros and cons.

That said, we proceed to the discussion of running times; these are valid in either the pure mathematical viewpoint or the floating point viewpoint.

If $\vec{u}$ and $\vec{v}$ are n-dimensional vectors and a is a scalar, then computing $a\vec{u}$, $\vec{v}+\vec{u}$, and $\vec{v} \bullet \vec{u}$ obviously requires time $O(n)$.

For a sparse vector $\vec{v}$, let us write $NZ(\vec{v})$ for the number of non-zero components of $\vec{v}$. Let $\vec{u}$ and $\vec{v}$ be sparse vectors and a be a scalar. Then, using the obvious algorithms, computing $a\vec{u}$ requires time $NZ(\vec{u})$. Computing $\vec{v}+\vec{u}$ and $\vec{v} \bullet \vec{u}$ requires time $NZ(\vec{v})+NZ(\vec{u})$. As discussed in section 2.7, the time requirement of indexing (that is, retrieving or setting $\vec{v}[i]$) depends on the details of the implementation; if a hash table is used, it requires expected constant time.

Multiplying an $m \times n$ matrix A times an n-dimensional vector $\vec{v}$ requires time $O(mn)$. If A and $\vec{v}$ are sparse then computing $A\vec{v}$ requires time $O(NZ(A) + NZ(\vec{v}))$.

Let A be an $m \times p$ matrix and let B be a $p \times n$ matrix. Computing the product $A \cdot B$ in the obvious way — that is, computing the dot product of each row of A with each column of B — involves computing mn dot products of p-dimensional vectors; thus, time $O(mpn)$. If $m = p = n$ (multiplying two square matrices) the time requirement[4] is $O(n^3)$.

It should also be noted that the multiplication algorithm is highly parallelizable; in the extreme case, if you have n^3 parallel processors, you can compute the product of two $n \times n$ matrices in time $O(\log n)$.

Surprisingly, there are actually methods known that are in principle faster for large matrices. As of the time of writing, the fastest known algorithm[5] for multiplying two $n \times n$ matrices requires time $O(n^{2.376})$. However, this algorithm and other algorithms that run in time faster than $O(n^3)$ are not used for two reasons. First, the constant factor associated with them is so large that they would only pay off over the simple algorithm when the matrices are too large to be effectively multiplied in any case. Second, they are numerically unstable.

A simple analysis of the algorithms presented in this chapter shows that, for n equations in n variables, SolveRowEchelon runs in time $O(n^2)$, and GaussianEliminate, SolveLinearEqns, and Inverse run in time $O(n^3)$. One can prove that, in principle, the faster matrix multiplication algorithm cited above can be used to construct algorithms for solving linear equations and for inverting a matrix that run in time $O(n^{2.376})$; these are not used in practice for the same reasons that the fast matrix multiplication algorithms are not used.

Exercises

Exercise 5.1

Solve the following system of linear equations, both by hand and in MATLAB. (Note: In solving systems of equations by hand, there is no reason to use the "maximum element row interchange" step. If anything, one should swap with the row which has the *minimal* non-zero value in the column, in order to keep the denominators of the fractions involved as small as possible.)

[4]Note that there is a discrepancy here from the usual way of describing algorithmic time requirements. Usually time requirements are described as a function of the size of the input to the algorithm; however, the size of the input in this problem is $O(n^2)$. If q is the size of the input, then the time requirement of this algorithm is $O(q^{3/2})$.

[5]D. Coppersmith and S. Winograd, "Matrix multiplication via arithmetic progressions," *J. Symbolic Computation* **9**, 1990, p. 251-280.

A.

$$\begin{array}{rcrcrcl} x & + & y & + & z & = & 0 \\ 2x & - & y & - & z & = & 2 \\ -x & + & y & - & z & = & 2 \end{array}$$

B.

$$\begin{array}{rcrcrcl} 2x & + & y & + & 2z & = & 3 \\ x & - & y & + & 3z & = & -2 \\ x & + & 3y & - & 3z & = & 2 \end{array}$$

C.

$$\begin{array}{rcrcrcrcl} w & + & x & + & y & - & z & = & 4 \\ 2w & + & 2x & - & y & & & = & 4 \\ w & - & x & - & y & - & z & = & -2 \\ & & x & + & y & + & z & = & 4 \end{array}$$

Exercise 5.2

The space of solutions to an underconstrained system equations $M\vec{X} = \vec{C}$ can be characterized in an expression of the form:

$$\{\vec{v} + a_1\vec{b}_1 + \ldots + a_k\vec{b}_k|$$

where $\vec{v}$ is one solution to the system; $\vec{b} \ldots \vec{b}_k$ are a basis for Null(M); and $a_1 \ldots a_k$ are scalar variables. For example the space of solutions to the single equation $x + y + z = 3$ can be characterized as:

$$\langle 1, 1, 1\rangle + a \cdot \langle 1, -1, 0\rangle + b \cdot \langle 1, 0, -1\rangle$$

By hand and using MATLAB, characterize the space of solutions to the following systems of linear equations.

A.

$$\begin{array}{rcrcrcl} x & + & y & - & z & = & 1 \\ x & + & y & + & z & = & 3 \end{array}$$

B.

$$\begin{array}{rcrcrcrcl} w & + & x & + & y & + & z & = & 5 \\ 2w & - & x & + & y & - & z & = & 0 \end{array}$$

C.

$$\begin{array}{rcrcrcrcl} w & + & x & + & y & + & z & = & 4 \\ 2w & - & x & + & y & - & z & = & 0 \\ w & - & x & - & 2y & + & z & = & -4 \end{array}$$

Programming Assignments

Assignment 5.1: Temperature distribution

In section 3.6.1 , application 18, we discuss finding steady-state temperature distribution inside an object by taking a collection of evenly spaced points, and asserting that the temperature at each point is the average of the temperature at the nearby points. It is assumed that the temperature at the border is fixed by some external constraint.

A. Write a MATLAB function `TempDist(TL,TR,TT,TB,N)` that sets up and solves this system of equations. Assume that TL is the temperature on the left side, TR is the temperature on the right side, TT is the temperature on top, TB is the temperature on the bottom. The function uses an $N \times N$ array of internal points. The function should return a $N \times N$ array T where $T[I, J]$ is the temperature at point I, J (I measured from the left, J measured from the top).

For example, for the particular example presented in the notes, the function call would be `TempDist(20,20,20,100,3)` and the value returned would be

$$\begin{bmatrix} 25.71 & 27.86 & 25.71 \\ 35.00 & 40.00 & 35.00 \\ 54.29 & 62.14 & 54.29 \end{bmatrix}$$

Note that the system of equations has N^2 equations in N^2 unknowns, thus a matrix of N^4 coefficients. Do not confuse the $N \times N$ array of temperatures with the $N^2 \times N^2$ array of coefficients.

B. Use MATLAB's plotting routines to plot the temperature as height over the two dimensional region.

Assignment 5.2: Curve interpolation

A. Using the technique described in section 3.6.1 , application 19, write a function `PolyInterpolate(M)`. The input parameter M is a $2 \times n$ matrix, where each column holds the x and y coordinates of one point. You may assume that no two points have the same x coordinate. The function should return the coefficients $a_{n-1} \ldots a_0$ of the $n-1$ degree polynomial $y = a_{n-1}x^{n-1} + \ldots + a_1 x_1 + a_0$ The function should also generate a plot of the curve with the input points, as in figure 3.4.

For instance, for the example in application 19, the function call `PolyInterpolate([-3,-1,0,2,4; 1,0,5,0,1])` should return the vector `[0.2167, -0.4333, -2.7167, 2.9333, 5.0000]` and generate the solid red curve of figure 3.4.

B. Write a function `SineInterpolate(M)` that interpolates a curve that is the sum of sinusoidal curves between input points. As in part A, the input parameter M is a $2 \times n$ where each column holds the x and y coordinates of one point. You may assume that n is an even number. The function should return the vector of coefficients $a_0, a_1 \ldots a_k, b_1 \ldots b_{k-1}$ such that the function

$$y(x) = a_0 + a_1 \sin(\pi x/2) + a_2 \sin(\pi x/4) + \ldots + a_k \sin(\pi x/2k) + b_1 \cos(\pi x/2) + b_2 \cos(\pi x/4) + \ldots + b_{k-1} \cos(\pi x/2(k-1))$$

interpolates the points in M. It should also plot the curve $y(x)$.

For instance, for the example in application 19, the function call `SineInterpolate([-3,-1,0,2,4; 1,0,5,0,1])` should return the vector `[0.2170, 1.6547,  0.9566, 2.3116, 2.6667]` and generate the dashed green curve of figure 3.4.

Assignment 5.3: Circuit Analysis

Write a MATLAB program `AnalyzeCircuit(C,R,V)` which carries out circuit analysis as described in section 3.6.1 application 17. The program should operate as follows. Let n be the number of nodes in the circuit; let b be the number of connections; let $q = n + b$. Assign the nodes indices $1 \ldots n$ where node 1 is ground (0 volts). Assign the branches indices $1 \ldots b$. Then the arguments are as follows:

- `C` is a $2 \times b$ array. `C[1,I]` and `C[2,I]` are the indices of the node at the tail and the head of branch `I`.

- `R` is a row vector of length b, where `R[I]` is the resistance of a resistor along branch `I`, and 0 if there is no resistor.
- `V` is a row vector of length b, where `V[I]` is a voltage source along branch `I`, and 0 if there is no voltage source.

You may assume that for every index `I` either `R[I]` or `V[I]` is non-zero, but not both.

In the example in figure 3.2, with nodes A, B, C associated with indices $1, 2, 3$, and the branches numbered as in the diagram, the input parameters are

$$C = \begin{bmatrix} 1 & 2 & 2 & 3 \\ 2 & 1 & 3 & 1 \end{bmatrix} \qquad R = \begin{bmatrix} 0 & 100 & 75 & 25 \end{bmatrix} \qquad V = \begin{bmatrix} 100 & 0 & 0 & 0 \end{bmatrix}$$

The program returns a vector $\vec{x}$ of dimension q where,

- For $i = 1 \ldots n$, $\vec{x}[i]$ is the voltage at node i.
- For $i = 1 \ldots q$, $\vec{x}[n + i]$ is the current through branch i.

Set up a $(q + 1) \times q$ matrix M and a $q + 1$-dimensional column vector c such that the system of linear equation $M\vec{x} = \vec{c}$ corresponds to the following constraints:

a. Ground. The voltage at the ground is equal to 0.

b. Voltage source. If $S[I, J] \neq 0$ then the voltage at J minus the voltage at I is equal $S[I, J]$.

c. Resistor. If $R[I, J] \neq 0$ then the voltage at I minus the voltage at J is equal to $R[I, J]$ times the current from I to J.

d. Kirchoff's current law. For each node, the sum of the currents on branches entering the node is equal to the sum of the currents on branches exiting the node. One of the equations is actually redundant (any one of them is redundant with respect to all the rest), but since the rank of the matrix is q, that doesn't do any harm.

Note that there is one equation of type (c); b equations of types (a) and (b) combined; and n equation of type (d), so in total there are $q + 1$ equations in q unknowns.

Now solve the system $M \cdot \vec{x} = \vec{c}$.

Chapter 6

Geometry

Many kinds of geometric concepts can be related to vectors and linear algebra. Therefore, linear algebra is important for computer applications that have to negotiate with physical space, including graphics, image processing, computer aided design and manufacturing, robotics, scientific computation, geographic information systems, and so on.

As we shall see, the fit between linear algebra and geometry is not perfect: central categories in linear algebra, such as the space of all linear transformations, are only moderately important geometrically, and central categories in geometry, such as polygons, do not correspond to anything at all natural in linear algebra. But where the two theories mesh together well, they can be extremely synergistic.

6.1 Arrows

The connection between geometry and linear algebra involves a somewhat abstract geometric entity which we will call an *arrow*.[1] An arrow has a specified length and direction, but not a specified position in the plane; it floats around without changing its length or rotating.[2] We will use boldface letters such at $\mathbf{p}$ for points and letters with thick arrows over them like $\vec{x}$ for arrows.

Points and arrows have four geometric operations defined on them (figure 6.1). Let $\mathbf{p}, \mathbf{q}, \mathbf{r}$ and $\mathbf{s}$ be points; let $\vec{a}$, $\vec{b}$, and $\vec{c}$ be arrows, and let t and w be numbers. Then

- The difference $\mathbf{q} - \mathbf{p}$ is an arrow; namely, the arrow whose head is at $\mathbf{q}$ when its tail is at $\mathbf{p}$.

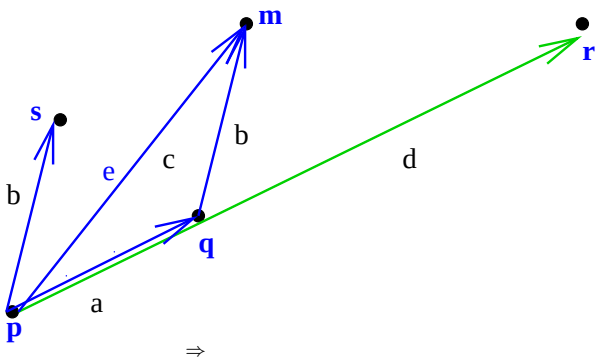
  The arrow $\mathbf{q} - \mathbf{p}$ is considered *the same* as the arrow $\mathbf{s} - \mathbf{r}$ if the ray from $\mathbf{r}$ to $\mathbf{s}$ and the ray from $\mathbf{p}$ to $\mathbf{q}$ have the same length and are parallel.

- The sum $\mathbf{p} + \vec{a}$ of a point plus an arrow is equal to the point $\mathbf{q}$ satisfying $\mathbf{q} - \mathbf{p} = \vec{a}$.

- The sum of two arrows $\vec{a} + \vec{b}$ is an arrow, equal to $((\mathbf{p} + \vec{a}) + \vec{b}) - \mathbf{p}$.

[1] An arrow is a kind of vector, under the general definition given in section 4.17; but there does not seem to be standard term for this specific geometric category.

[2] The problem in explaining geometric vector theory is that there is no really good way to draw or visualize an arrow. You can draw all arrows with their tail at the origin, but then it is hard to explain the difference between an arrow and the point at the head of the arrow. Or you can draw "floating" arrows, with their tails at some other point, but then it is hard to explain that the arrow from, say, $\langle 1, 3\rangle$ to $\langle 2, 5\rangle$ is the same as the arrow from $\langle 3, 2\rangle$ to $\langle 4, 4\rangle$ since, pictorially, it is obviously a different thing. And it is hard to visualize a geometric arrow as a physical arrow that can be moved around the plane, because it is hard to imagine why you aren't allowed to rotate it.



$$\vec{a} = \mathbf{q} - \mathbf{p} = \mathbf{m} - \mathbf{s}$$
$$\mathbf{q} = \mathbf{p} + \vec{a}.$$
$$\vec{b} = \mathbf{s} - \mathbf{p}$$
$$\vec{c} = \mathbf{m} - \mathbf{p} = \vec{b} + \vec{a}$$
$$\vec{d} = 3 \cdot \vec{a}.$$

Figure 6.1: Operations on points and arrows

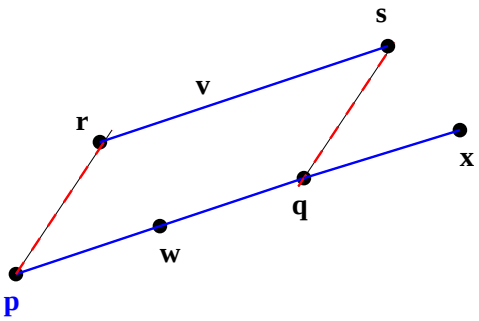


Figure 6.2: The differences $\mathbf{q} - \mathbf{p}$, $\mathbf{s} - \mathbf{r}$ and $\mathbf{x} - \mathbf{w}$ are the same arrow $\vec{v}$

- The product $t \cdot \vec{a}$ is an arrow. Let $\vec{a} = \mathbf{q} - \mathbf{p}$. Then $t \cdot \vec{a} = \mathbf{r} - \mathbf{p}$, where $\mathbf{p}, \mathbf{q}$, and $\mathbf{r}$ are collinear; $\mathrm{d}(\mathbf{p}, \mathbf{r}) = |t| \cdot \mathrm{d}(\mathbf{p}, \mathbf{q})$ and [if $t > 0$ then $\mathbf{r}$ and $\mathbf{q}$ are on the same side of $\mathbf{p}$; if $t < 0$ then $\mathbf{r}$ and $\mathbf{q}$ are on opposite sides of $\mathbf{p}$].

The following geometric rules establish that arrows are vectors, in the abstract sense (section 4.17):

$$\vec{a} + \vec{b} = \vec{b} + \vec{a}$$
$$(\vec{a} + \vec{b}) + \vec{c} = \vec{a} + (\vec{b} + \vec{c}).$$
$$(\mathbf{p} + \vec{a}) + \vec{b} = \mathbf{p} + (\vec{a} + \vec{b}).$$
$$t \cdot (\vec{a} + \vec{b}) = t \cdot \vec{a} + t \cdot \vec{b}.$$
$$(t + w) \cdot \vec{a} = t \cdot \vec{a} + w \cdot \vec{a}.$$
$$(t \cdot w) \cdot \vec{a} = t \cdot (w \cdot \vec{a})$$

A point $\mathbf{r}$ lies on the line $\mathbf{pq}$ if the arrows $\mathbf{q} - \mathbf{p} = t(\mathbf{r} - \mathbf{p})$ for some value of t. Therefore the set of all points on the line connecting $\mathbf{p}$ and $\mathbf{q}$ is given by $\{\mathbf{p} + t \cdot (\mathbf{q} - \mathbf{p}) | t \in \mathbb{R}\}$.

6.2 Coordinate systems

Suppose that we have a collection of points in the plane; think of these as relatively small, fixed, physical things, like thumbtacks in a bulletin board, or lampposts in a city. We want to record the position of these in a database or a gazeteer. The standard solution, of course, is to use coordinates in a coordinate system. We have already discussed this in application 1 of chapter 2, but it will be helpful to go over it again, very carefully this time.

A coordinate system for the plane consists of a point $\mathbf{o}$, the origin; a unit distance d_1 (e.g. a meter or a mile); and two orthogonal arrows $\vec{x}$ and $\vec{y}$ of length d_1. The coordinate vector of an arrow $\vec{a}$ with respect to this coordinate system is the pair of numbers $\langle s, t \rangle$ such that $\vec{a} = s \cdot \vec{x} + t \cdot \vec{y}$. The coordinate vector of a point $\mathbf{p}$ with respect to this coordinate system is the pair of numbers $\langle s, t \rangle$ such that $\mathbf{p} = \mathbf{o} + s \cdot \vec{x} + t \cdot \vec{y}$. (Figure 6.3). If $\mathcal{C}$ is a coordinate system, $\mathbf{p}$ is a point and $\vec{v}$ is an arrow, then we will write "Coords($\mathbf{p}, \mathcal{C}$)" and "Coords($\vec{v}, \mathcal{C}$)" to mean the coordinates of $\mathbf{p}$ and $\vec{v}$ in system $\mathcal{C}$.

The x-axis of the coordinate system is the line $\{\mathbf{o} + t\vec{x} | t \in \mathbb{R}\}$, and the y-axis is the line $\{\mathbf{o} + t\vec{y} | t \in \mathbb{R}\}$.

The coordinates of $\mathbf{p}$ can be measured by dropping perpendiculars from $\mathbf{p}$ to point $\mathbf{a}$ on the x-axis and to point $\mathbf{b}$ on the y-axis. The coordinate $\mathbf{p}[1]$ is then $\pm d(\mathbf{a}, \mathbf{o})/d_1$, with a positive sign if $\mathbf{a}$ and $\mathbf{o} + \vec{x}$ are on the same side of $\mathbf{o}$ and a negative sign if they are on opposite sides. Likewise, the coordinate $\mathbf{p}[2]$ is $\pm d(\mathbf{b}, \mathbf{o})/d_1$, with the corresponding rule for sign.

If L is any distance, then the measure of L in $\mathcal{C}$, $\mathrm{Coords}(L, \mathcal{C}) = L/d_1$.

In three dimensions, a coordinate system includes a third arrow $\vec{z}$ which is orthogonal to both $\vec{x}$ and $\vec{y}$. The coordinates of an arrow and of a point are defined and measured analogously.

It is then a geometric theorem, easily proven, that the operations on points and arrows correspond, in the obvious way, to the operations of the same name on their coordinate vectors; e.g.
$\mathrm{Coords}(\mathbf{p} + \vec{v}, \mathcal{C}) = \mathrm{Coords}(\mathbf{p}, \mathcal{C}) + \mathrm{Coords}(\vec{v}, \mathcal{C})$.

I have belabored this at such length in order to emphasize the distinction between the geometric domain of points and arrows and the geometric operations on them, and the numeric domain of coordinate vectors and the arithmetic operations on *them*, and to emphasize that the geometric

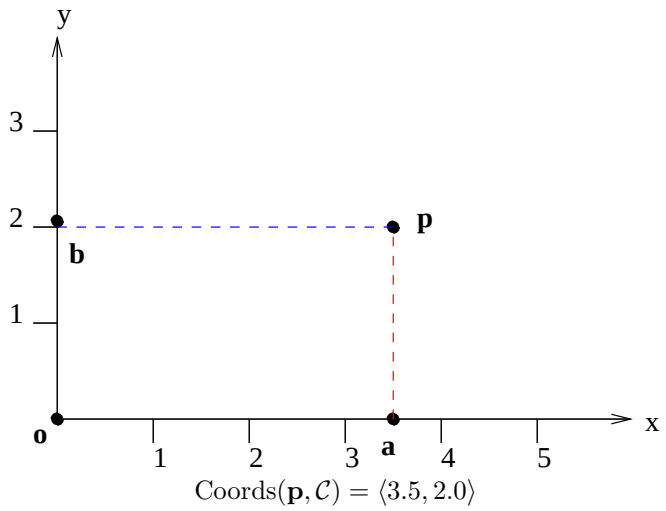


Figure 6.3: Coordinate System

operations do what they do on the geometric objects regardless of how we choose to represent them as numeric vectors. In the text below, I will follow the usual practice, convenient though imprecise, of conflating the geometric objects with their coordinate system representation; e.g. writing $\vec{v} \bullet \vec{u}$ where what I really mean is Coords$(\vec{v}, \mathcal{C}) \bullet$ Coords$(\vec{u}, \mathcal{C})$. I will explicitly mention the coordinate system only in cases where there is more than one coordinate system under consideration, particularly in chapter 7.

6.3 Simple geometric calculations

The power of the coordinate system approach to geometry is that all kinds of geometric concepts and calculations can now be expressed in terms of the coordinates in the entities involved. In this book, we confine ourselves exclusively to those geometric concepts and operations that turn out to be closely related to concepts and operations of linear algebra.

6.3.1 Distance and angle

We have already in chapter 2 discussed two geometric formulas that use the dot product:

- The length of arrow $\vec{v}$ is $\sqrt{\vec{v} \bullet \vec{v}} = |\vec{v}|$. The distance between points $\mathbf{p}$ and $\mathbf{q}$ is $\sqrt{(\mathbf{p}-\mathbf{q}) \bullet (\mathbf{p}-\mathbf{q})} = |\mathbf{p}-\mathbf{q}|$.
  Example: The length of arrow $\langle 1, 1\rangle$ is $\sqrt{1^2+1^2} = \sqrt{2}$. The distance from $\langle 0, 4, 3\rangle$ to $\langle -1, 2, 4\rangle$ is $\sqrt{(-1-0)^2+(2-4)^2+(4-3)^2} = \sqrt{6}$.
- The angle ϕ between arrows $\vec{u}$ and $\vec{v}$ satisfies $\cos(\phi) = \vec{u} \bullet \vec{v}/|\vec{u}| \cdot |\vec{v}|$. In particular, if $\vec{v}$ is orthogonal to $\vec{u}$, then $\phi = \pi/2$, $\cos(\phi) = 0$ so $\vec{u} \bullet \vec{v} = 0$.
  Example: If $\vec{u} = \langle 1, 3\rangle$ and $\vec{v} = \langle 4, 1\rangle$ then $\cos(\phi) = \vec{u} \bullet \vec{v}/|\vec{u}| \cdot |\vec{v}| = 7/\sqrt{10}\sqrt{17} = 0.5369$ so $\phi = \cos^{-1}(0.5369) = 1.0041$ radians $= 57.53°$.

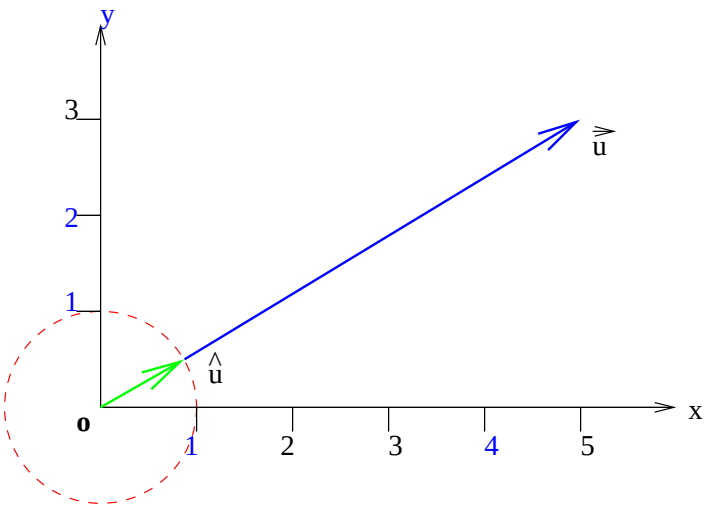


Figure 6.4: Arrows and their directions

The set of points $\mathbf{p}$ that are distance r from center $\mathbf{c}$ is, the circle, in two dimensions, or the sphere, in three dimensions, of radius r and center $\mathbf{c}$. It can be represented by the equation $|\mathbf{p}-\mathbf{c}| = r$, or equivalently $(\mathbf{p}-\mathbf{c}) \bullet (\mathbf{p}-\mathbf{c}) = r^2$. A point $\mathbf{p}$ is inside this circle if $(\mathbf{p}-\mathbf{c}) \bullet (\mathbf{p}-\mathbf{c}) < r^2$. It is outside if $(\mathbf{p}-\mathbf{c}) \bullet (\mathbf{p}-\mathbf{c}) > r^2$.

6.3.2 Direction

A *direction* in two-space or three-space can be taken to be a *unit* arrow; that is, an arrow of length d_0. These are often written with a hat over them, such as $\hat{u}$. The *direction* of non-zero arrow $\vec{u}$, denoted $\mathrm{Dir}(\vec{u})$ or $\hat{u}$ is defined as $(d_0/|\vec{u}|) \cdot \vec{u}$; thus, in a coordinate system $\mathcal{C}$ with unit length d_0 we have $\mathrm{Coords}(\vec{u}, \mathcal{C}) = \mathrm{Coords}(|\vec{u}|, \mathcal{C}) \cdot \mathrm{Coords}(\hat{u}, \mathcal{C})$

Arrows $\vec{u}$ and $\vec{v}$ are *parallel* if $\vec{v} = c\vec{u}$ for some $c \neq 0$; equivalently $\mathrm{Dir}(\vec{u}) = \pm\,\mathrm{Dir}(\vec{v})$.

Example: If $\vec{u} = \langle 3, 4\rangle$, then, since $|\vec{u}| = 5$ we have $\hat{u} = \mathrm{Dir}(\vec{u}) = \langle 3/5, 4/5\rangle$. If $\vec{v} = \langle 1, 1\rangle$ then, since $|\vec{v}| = \sqrt{2}$, we have $\hat{v} = \mathrm{Dir}(\vec{v}) = \langle 1/\sqrt{2}, 1/\sqrt{2}\rangle$. The vector $\langle 9, 12\rangle = 3\vec{u} = 15\hat{u}$ and the vector $\langle -6, -8\rangle = -2\vec{u} = -10\hat{u}$ are parallel to $\vec{u}$ (Figure 6.4).

If $\vec{v} = c\vec{u}$ then $\vec{v}$ and $\vec{u}$ are linearly dependent, so the matrix whose rows are $\vec{v}, \vec{u}$ has rank 1.

In two dimensions, let $\vec{v}$ be the arrow with coordinates $\langle V_x, V_y\rangle$. The vector that results from rotating $\vec{v}$ by 90° is $\langle -V_y, V_x\rangle$ for a counter-clockwise rotation (assuming the usual layout of x and y axes) and $\langle V_y, -V_x\rangle$ for a clockwise rotation. It is trivial to check that these have the same length as $\vec{v}$ and are orthogonal to $\vec{v}$.

6.3.3 Lines in two-dimensional space

As we said above, the line from $\mathbf{p}$ to $\mathbf{q}$ is the set of points $\{\mathbf{p} + t \cdot (\mathbf{q}-\mathbf{p}) \,|\, t \in \mathbb{R}\}$. In two dimensions, another way to characterize the line from $\mathbf{p}$ to $\mathbf{q}$ is as follows: Let $\vec{v} = \mathbf{q} - \mathbf{p}$ and let $\vec{w}$ be the arrow that is orthogonal to $\vec{v}$. Let $\mathbf{s}$ be any point in two-space; then there exist a and b such that $\mathbf{s} = \mathbf{p} + a\vec{v} + b\vec{w}$. By the above definition, $\mathbf{s}$ is on the line $\mathbf{pq}$ if and only if $b = 0$. But note that

$$\mathbf{s} \bullet \vec{w} = (\mathbf{p} + a\vec{v} + b\vec{w}) \bullet \vec{w} = \mathbf{p} \bullet \vec{w} + a\vec{v} \bullet \vec{w} + b\vec{w} \bullet \vec{w} = \mathbf{p} \bullet \vec{w} + b\vec{w} \bullet \vec{w}$$

So if $b = 0$ then $\mathbf{s} \bullet \vec{w} = \mathbf{p} \bullet \vec{w}$ and conversely. Thus a point $\mathbf{s}$ is on the line $\mathbf{p},\mathbf{q}$ if and only if it satisfies $\mathbf{s} \bullet \vec{w} = \mathbf{p} \bullet \vec{w}$ where $\vec{w}$ is a vector orthogonal to $\mathbf{q} - \mathbf{p}$. Note that $\mathbf{p} \bullet \vec{w}$ is a constant, independent of $\mathbf{s}$.

Note also that if x and y are variables representing the coordinates of $\mathbf{s}$ then this is a single linear equation in x and y: $\vec{w}[1] \cdot x + \vec{w}[2] \cdot y = \mathbf{p} \bullet \vec{w}$.

The line $\mathbf{L} = \{\mathbf{s} \mid \mathbf{s} \bullet \vec{w} = c\}$ divides two-dimensional space into three regions: the line itself, points on one side, and points on the other. A point $\mathbf{a}$ on the $\vec{w}$ side of $\mathbf{L}$ satisfies $\mathbf{a} \bullet \vec{w} > c$; a point $\mathbf{b}$ on the opposite side satisfies $\mathbf{b} \bullet \vec{w} < c$. The two sides of the line are called the *half-spaces* defined by the line. A *closed half-space* includes the line itself, while an *open half-space* excludes the line.

Note that we now have three ways to represent a line:
(a) as a pair of points $\mathbf{p},\mathbf{q}$;
(b) in parameterized form $\{\mathbf{p} + t\vec{v} \mid t \in \mathbb{R}\}$, where $\vec{v} = \mathbf{q} - \mathbf{p}$;
(c) as the solutions to the linear equation $\{\mathbf{s} \mid \mathbf{s} \bullet \vec{w} = c\}$ where $\vec{w}$ is orthogonal to $\vec{v}$ and where c is the constant $\mathbf{p} \bullet \vec{w}$.
With each of these, there is a method to carry out a simple operation, such as checking whether a point $\mathbf{s}$ is on the line:

- $\mathbf{s}$ is on line $\mathbf{pq}$ if $\mathbf{s} - \mathbf{p}$ is parallel to $\mathbf{s} - \mathbf{q}$, which holds if the matrix with these two vectors as rows has rank 1.
- $\mathbf{s}$ is on the line $\{\mathbf{p} + t\vec{v} \mid t \in \mathbb{R}\}$ if the pair of linear equations
$$\vec{v}[1]t = \mathbf{s}[1] - \mathbf{p}[1]$$
$$\vec{v}[2]t = \mathbf{s}[2] - \mathbf{p}[2]$$
has a solution. (This is a pair of linear equations in the single unknown t.)
- $\mathbf{s}$ is on the line $\{\mathbf{s} \mid \mathbf{s} \bullet \vec{w} = c\}$ if $\mathbf{s} \bullet \vec{w} = c$.

Example (figure 6.5): Let $\mathbf{p}$ be the point $\langle 1, 2\rangle$ and $\mathbf{q}$ be the point $\langle 4, 3\rangle$. Then $\vec{v} = \mathbf{q} - \mathbf{p} = \langle 3, 1\rangle$. So the line $\mathbf{pq}$ can be expressed as the set $\{\mathbf{p} + t\vec{v} | t \in \mathbb{R}\} = \{\langle 1 + 3t, 2 + t\rangle | t \in \mathbb{R}\}$ The arrow $\vec{w} = \langle -1, 3\rangle$ is orthogonal to $\vec{v}$. So the line $\mathbf{pq}$ can also be expressed as the set $\{\mathbf{s} | \mathbf{s} \bullet \vec{w} = \mathbf{p} \bullet \vec{w}\}$; that is $\{\langle x, y\rangle | -x + 3y = 5\}$.

We can check that the point $\mathbf{s} = \langle 7, 4\rangle$ is on the line either by checking

a. The matrix
$$\begin{bmatrix} \mathbf{s} - \mathbf{p} \\ \mathbf{s} - \mathbf{q} \end{bmatrix} = \begin{bmatrix} 6 & 2 \\ 3 & 1 \end{bmatrix}$$
has rank 1.

b. The pair of equations $\vec{v}t = \mathbf{s} - \mathbf{p}$, that is,
$$3t = (7 - 1)$$
$$t = (4 - 2)$$
has a solution (namely $t = 2$).

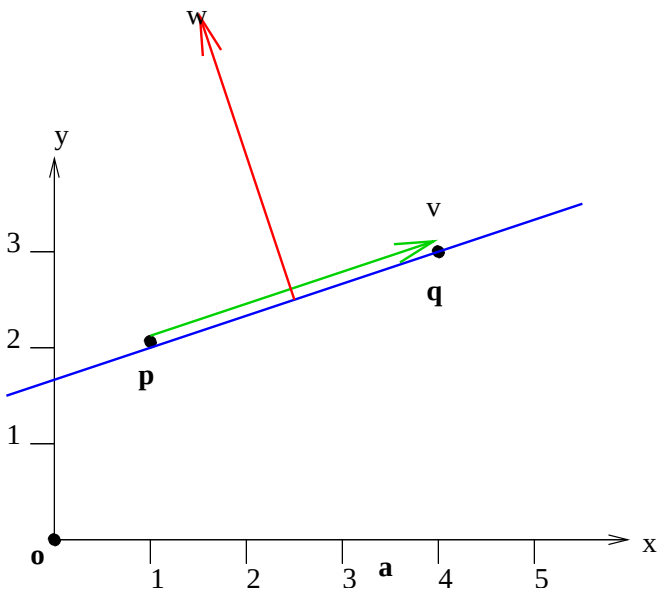


Figure 6.5: Representations of a line in two-space

c. The dot product $\mathbf{s} \bullet \vec{w} = \mathbf{p} \bullet \vec{w}$. That is, $\langle 7, 4\rangle \bullet \langle -1, 3\rangle = \langle 1, 2\rangle \bullet \langle -1, 3\rangle = 5$.

The point $\langle 2, 4\rangle$ is on the $\vec{w}$ side of $\mathbf{pq}$; thus $-1 \cdot 2 + 3 \cdot 4 = 10 > 5$. The point $\langle 2, 2\rangle$ is on the $-\vec{w}$ side of $\mathbf{pq}$; thus $-1 \cdot 2 + 3 \cdot 2 = 4 < 5$.

6.3.4 Lines and planes in three-dimensional space

The situation is similar in three-dimensional space. It is a little more complicated, though; some of the properties of lines in two-space carry over to lines in three-space; some properties carry over to planes in three-space; and some things are simply different.

Planes in three-space

In three-dimensions, a point $\mathbf{s}$ is in the plane containing points $\mathbf{p}$, $\mathbf{q}$ and $\mathbf{r}$ if $\mathbf{s} - \mathbf{p}$ is a linear sum of $\mathbf{q} - \mathbf{p}$ and $\mathbf{r} - \mathbf{p}$. That is, let $\vec{u} = \mathbf{q} - \mathbf{p}$ and $\vec{v} = \mathbf{r} - \mathbf{p}$; then the plane is the set of points $\{\mathbf{p} + a \cdot \vec{u} + b \cdot \vec{v} \mid a, b \in \mathbb{R}\}$.

Again, there is an alternative representation using the dot product. Let $\vec{w}$ be a vector that is orthogonal to both $\vec{u}$ and $\vec{v}$. Let $\mathbf{s}$ be any point in three space; then there exist a, b and c such that $\mathbf{s} = \mathbf{p} + a\vec{u} + b\vec{v} + c\vec{w}$. $\mathbf{s}$ is in the plane $\mathbf{pqr}$ if and only if $c = 0$. But

$$\mathbf{s} \bullet \vec{w} = \mathbf{p} \bullet \vec{w} + a\vec{u} \bullet \vec{w} + b\vec{v} \bullet \vec{w} + c\vec{w} \bullet \vec{w} = \mathbf{p} \bullet \vec{w} + c\vec{w} \bullet \vec{w}$$

So $c = 0$ if and only if $\mathbf{s} \bullet \vec{w} = \mathbf{p} \bullet \vec{w}$. Thus, the plane is the set of points $\{\mathbf{s} \mid \mathbf{s} \bullet \vec{w} = \mathbf{p} \bullet \vec{w}\}$. Note that this is a single linear equation in three variables: $\vec{w}[1] \cdot \mathbf{s}[1] + \vec{w}[2] \cdot \mathbf{s}[2] + \vec{w}[3] \cdot \mathbf{s}[3] = \vec{w} \cdot \mathbf{p}$. (The values of $\vec{w}$ and $\mathbf{p}$ are known; the coordinates of $\mathbf{s}$ are variables.)

This plane divides the rest of three-space into the two open half-spaces $\{\mathbf{s} \mid \mathbf{s} \bullet \vec{w} > \mathbf{p} \bullet \vec{w}\}$ and $\{\mathbf{s} \mid \mathbf{s} \bullet \vec{w} < \mathbf{p} \bullet \vec{w}\}$.

Finding a vector $\vec{w}$ perpendicular to $\vec{u}$ and $\vec{v}$ is trickier than in two-space. A simple formula for this is the *cross-product* $\vec{u} \times \vec{v}$ which is computed as follows: Let the coordinates of $\vec{u}$ and $\vec{v}$ be $\langle u_x, u_y, u_z\rangle$ and $\langle v_x, v_y, v_z\rangle$. Then the coordinates of the cross-product $\vec{w}$ are given by

$$\vec{w} = \vec{u} \times \vec{v} = \langle u_y v_z - u_z v_y, u_z v_x - u_x v_z, u_x v_y - u_y v_x\rangle$$

It is straightforward to check that $\vec{w} \bullet \vec{u} = 0$ and $\vec{w} \bullet \vec{v} = 0$, and that if $\vec{u}$ and $\vec{v}$ are not parallel, then $\vec{u} \times \vec{v} \neq \vec{0}$.

Example Let $\mathbf{p} = \langle 0, 1, 1\rangle$, $\mathbf{q} = \langle 1, 2, 1\rangle$, $\mathbf{r} = \langle 2, 0, 0\rangle$. Then $\vec{u} = \mathbf{q} - \mathbf{p} = \langle 1, 1, 0\rangle$ and $\vec{v} = \mathbf{r} - \mathbf{p} = \langle 2, -1, -1\rangle$. Therefore any point of the form $\mathbf{p} + a\vec{u} + b\vec{v}$ is in the plane; e.g. for $a = 2, b = 2$ this is the point $\langle 6, 1, -1\rangle$. For $a = 0, b = -1$ this is $\langle -2, 2, 2\rangle$. The cross-product $\vec{w} = \vec{u} \times \vec{v} = \langle -1, 1, -3\rangle$. So a point $\mathbf{s}\langle x, y, z\rangle$ on the plane satisfies the equation $\mathbf{s} \bullet \vec{w} = \mathbf{p} \bullet \vec{w}$; that is, $-x + y - 3z = -2$. The open half-spaces are given by $-x + y - 3z > 2$ and $-x + y - 3z < 2$.

Another way to determine whether point $\mathbf{s}$ lies in the same plane as $\mathbf{p}, \mathbf{q}, \mathbf{r}$ is to observe that, if so, $\mathbf{s} - \mathbf{p}$, $\mathbf{s} - \mathbf{q}$, and $\mathbf{s} - \mathbf{r}$ are linearly dependent. Therefore the matrix with these three vectors as rows has rank at most 2.

Lines in three-space

As in two-space, the line $\mathbf{pq}$ is the set of points $\{\mathbf{p} + t\vec{v} \mid t \in \mathbb{R}\}$ where $\vec{v} = \mathbf{q} - \mathbf{p}$.

A line in three-space is the solution space of a *pair* of linear equations. Let $\vec{w}$ and $\vec{u}$ be two non-parallel arrows that are both orthogonal to $\vec{v}$. Let $\mathbf{s}$ be any point in three-space; then there exists scalars a, b and c such that $\mathbf{s} = \mathbf{p} + a\vec{v} + b\vec{u} + c\vec{w}$. Now we have

$$\mathbf{s} \bullet \vec{u} = (\mathbf{p} + a\vec{v} + b\vec{u} + c\vec{w}) \bullet \vec{u} = \mathbf{p} \bullet \vec{u} + (b\vec{u} + c\vec{w}) \bullet \vec{u} \tag{6.1}$$

Likewise

$$\mathbf{s} \bullet \vec{w} = \mathbf{p} \bullet \vec{w} + (b\vec{u} + c\vec{w}) \bullet \vec{w} \tag{6.2}$$

Clearly if $b = c = 0$ then we have the pair of equations (6.3) $\mathbf{s} \bullet \vec{u} = \mathbf{p} \bullet \vec{u}$ and (6.4) $\mathbf{s} \bullet \vec{w} = \mathbf{p} \bullet \vec{w}$. Less obviously, the converse also holds. We know that (6.1) and (6.2) hold for all $\mathbf{s}$. Suppose that (6.3) and (6.4) also holds for some particular $\mathbf{s}$. Then, subtracting (6.3) from (6.1) and (6.4) from (6.2) we get the pair of equations $(b\vec{u} + c\vec{w}) \bullet \vec{u} = 0$ and $(b\vec{u} + c\vec{w}) \bullet \vec{w} = 0$. But since the arrow $b\vec{u} + c\vec{w}$ is in the same plane as $\vec{u}$ and $\vec{w}$, it can be orthogonal to both $\vec{u}$ and $\vec{w}$ only if $b\vec{u} + c\vec{w} = \vec{0}$; since $\vec{u}$ and $\vec{w}$ are non-parallel, that means that $b = c = 0$.

We have shown that point $\mathbf{s}$ is on line $\mathbf{pq}$ if and only $\mathbf{s} \bullet \vec{u} = \mathbf{p} \bullet \vec{u}$ and $\mathbf{s} \bullet \vec{w} = \mathbf{p} \bullet \vec{w}$. Let the coordinates of $\mathbf{s}$ be $\langle x, y, z\rangle$; then $\mathbf{s}$ is on the line from $\mathbf{p}$ to $\mathbf{q}$ just if x, y, z satisfy the *two* linear equations,

$$\begin{array}{ccccccc} \vec{u}[1]x & + & \vec{u}[2]y & + & \vec{u}[3]z & = & \vec{u} \bullet \mathbf{p} \\ \vec{w}[1]x & + & \vec{w}[2]y & + & \vec{w}[3]z & = & \vec{w} \bullet \mathbf{p} \end{array}$$

To find two non-parallel vectors $\vec{u}$ and $\vec{w}$ that are orthogonal to $\vec{v}$, one can proceed as follows: Let i be an index such that $\vec{v}[i] \neq 0$ and let j and k be the other two indices. Then we can define $\vec{u}$ so that $\vec{u}[i] = \vec{v}[j]; \vec{u}[j] = -\vec{v}[i]; \vec{u}[k] = 0$; and define $\vec{w}$ so that $\vec{w}[i] = \vec{v}[k]; \vec{w}[k] = -\vec{v}[i]; \vec{w}[j] = 0$.

In some cases, it is useful to require also that $\vec{u}$ and $\vec{w}$ be perpendicular to one another; in that case, define $\vec{u}$ as above and $\vec{w}$ as the cross-product $\vec{v} \times \vec{u}$.

Example: Let $\mathbf{p} = \langle 1, 1, 1\rangle$ and let $\mathbf{q} = \langle 3, 4, 5\rangle$. Then $\vec{v} = \mathbf{q} - \mathbf{p} = \langle 2, 3, 4\rangle$. Choosing $i = 3, j = 1, k = 2$ we have $\vec{u} = \langle -4, 0, 2\rangle$ and $\vec{w} = \langle 0, -4, 3\rangle$. So the line $\mathbf{pq}$ is defined by the two equations $\mathbf{s} \bullet \vec{u} = \mathbf{p} \bullet \vec{u}$; that is, $-4x + 2z = -2$; and $\mathbf{s} \bullet \vec{w} = \mathbf{p} \bullet \vec{w}$; that is, $-4y + 3z = -1$.

Again we have three formats for representing a line, and each format has a different associated method for checking whether the point is on the line.

- A line is determined by two points $\mathbf{pq}$. Point $\mathbf{s}$ is on the line if the 2×3 matrix with rows $\mathbf{s} - \mathbf{p}$, $\mathbf{s} - \mathbf{q}$ has rank 1.
- A line is expressed in parameterized form $\{\mathbf{p} + t\vec{v} | t \in \mathbb{R}\}$ where $\vec{v} = \mathbf{q} - \mathbf{p}$. Point $\mathbf{s}$ is on the line if the system of three equations in one variable $\vec{v}t = \mathbf{s} - \mathbf{p}$ has a solution.
- A line is expressed as a pair of linear equations $\mathbf{s} \bullet \vec{u} = a$ and $\mathbf{s} \bullet \vec{w} = b$. Point $\mathbf{s}$ is on the line if it satisfies the two equations.

6.3.5 Identity, incidence, parallelism, intersection

The previous section presented three kinds of representations for lines in two-space and lines and planes in three-space:

- Representation in terms of points. A line is represented in terms of two points on the line; a plane is represented in terms of three non-collinear points in the plane.
- Parameterized representation. A line is represented in the form $\mathbf{p} + t\vec{v}$. A plane is represented in the form $\mathbf{p} + a\vec{v} + b\vec{w}$, where $\vec{v}$ and $\vec{w}$ are non-parallel vectors parallel to the plane.
- Linear equations. A line in two-space or a plane in three-space is represented in terms of a single linear equation $\mathbf{s} \bullet \vec{w} = \mathbf{p} \bullet \vec{w}$, where $\vec{w}$ is the normal to the plane. A line in three-space is represented in terms of a pair of linear equations $\mathbf{s} \bullet \vec{w} = \mathbf{p} \bullet \vec{w}$, $\mathbf{s} \bullet \vec{u} = \mathbf{p} \bullet \vec{u}$, where $\vec{w}$ and $\vec{u}$ are not parallel and are orthogonal to the line.

None of these representations is unique; that is, for any geometric object (line/plane), and any style of representations, there are multiple ways to represent the same object. For instance the equations $x + 2y = 2$ and $2x + 4y = 4$ represent the same line in the plane, and similarly for the other representational styles. This is to some extent unavoidable; there is no method for representing lines or planes in terms of numerical parameters that is entirely non-problematic. For instance, lines in the plane are often represented in the form $y = mx + b$, which does give a unique representation for lines not parallel to the y-axis, but requires that lines that are parallel to the y-axis be given a different kind of representation $x = a$. (Also, this representation is unstable for lines that are nearly parallel to the y-axis.)

With each kinds of these objects, and with each of these representations, there are a number of basic problems to be solved:

- Identity: Do two representations represent the same object?
- Conversion: Convert the representation of an object in one format to another format.
- Incidence: Does a point lie on a line or plane? Does a line lie in a plane?
- Generation: Generate a point that lies on a given line or plane, or a line that lies in a given plane.

- Parallelism: Are two objects parallel, or do they intersect, or (for two lines in three-space) are they skew?
- Intersection: If two objects do intersect, find their intersection.

We have discussed all forms of problem of the incidence of a point on a line or plane in the previous section. The remaining problems are likewise straightforward. In general, the methods involved fall into one of four categories, in increasing order of complexity.

- Trivial. For instance, if plane $P1$ is represented by equation $E1$ and plane $P2$ is represented by equation $E2$ then their intersection is the line represented by the pair of equations $\{E1, E2\}$.
- Simple arithmetic. For instance, if line L is represented in terms of the coordinates of two points $\mathbf{p}$ and $\mathbf{q}$ that lie on L, then the conversion to parameterized form is $\mathbf{p} + t(\mathbf{q} - \mathbf{p})$.
- Computing rank. For instance, two planes characterized parametrically as $\mathbf{p} + a\vec{v} + b\vec{w}$ and $\mathbf{q} + c\vec{u} + d\vec{x}$ are parallel or identical if the matrix with rows $\vec{v}, \vec{w}, \vec{u}, \vec{x}$ has rank 2.
- Solving systems of linear equations (1, 2, or 3 equations in 1, 2, or 3 variables). For instance, finding the intersection of two lines, or finding the intersection of a line and a plane, in any representation, involves solving a system of equations (assuming that the point answer is to be represented in terms of coordinates).

6.3.6 Projections

The *projection* of a point $\mathbf{a}$ onto a plane or line X, denoted "Proj$(\mathbf{a}, X)$", is the point $\mathbf{q}$ in X that is closest to $\mathbf{a}$. The distance from $\mathbf{a}$ to X is, by definition, the distance from $\mathbf{a}$ to $\mathbf{q}$. The point $\mathbf{q}$ is the only point on X such that the line from $\mathbf{a}$ to $\mathbf{q}$ is orthogonal to X. Proof (figure 6.6): Let $\mathbf{b}$ be any point on $\mathbf{x}$ and draw the circle C centered at $\mathbf{a}$ with radius $\mathbf{ab}$. Then the following statements are equivalent:

$\mathbf{b}$ =Proj$(\mathbf{a}, X)$.
$\mathbf{b}$ is the closest point in X to $\mathbf{a}$.
$\mathbf{b}$ is on the boundary of C, and every other point on X is outside C.
X is tangent to C at $\mathbf{b}$.
X is orthogonal to the radius of C, $\mathbf{ab}$.

Suppose X is the line $\{\mathbf{p} + t\vec{v} | t \in \mathbb{R}\}$. Let $\hat{v} = \text{Dir}(\vec{v})$. Then $\mathbf{q}$= Proj$(\mathbf{a}, X) = \mathbf{p} + ((\mathbf{a} - \mathbf{p}) \bullet \hat{v}) \cdot \hat{v}$. Proof:

$$(\mathbf{a} - \mathbf{q}) \bullet \hat{v} = (\mathbf{a} - (\mathbf{p} + ((\mathbf{a} - \mathbf{p}) \bullet \hat{v}) \cdot \hat{v})) \bullet \hat{v} = (\mathbf{a} - \mathbf{p}) \bullet \hat{v} - (\mathbf{a} - \mathbf{p}) \bullet \hat{v} = 0$$

So $\mathbf{a} - \mathbf{q}$ is orthogonal to X, so, by the above proof, $\mathbf{q}$=Proj$(\mathbf{a}, X)$.

In three space, suppose X is the plane $\{\mathbf{p} + s\vec{u} + t\vec{v} \ | s, t \in \mathbb{R}\}$ where $\vec{u}$ and $\vec{v}$ are orthogonal. Let $\hat{u} = \text{Dir}(\vec{u})$ and $\hat{v} = \text{Dir}(\vec{v})$. Then Proj$(\mathbf{a}, X) = \mathbf{p} + ((\mathbf{a} - \mathbf{p}) \bullet \hat{v}) \cdot \hat{v} + ((\mathbf{a} - \mathbf{p}) \bullet \hat{u}) \cdot \hat{u}$. The proof is essentially identical.

6.4 Geometric transformations

One of the most important applications of linear algebra to geometry is the use of linear transformation to represent some of the ways in which objects or images can be moved around in space. This has many computer science applications, such as:

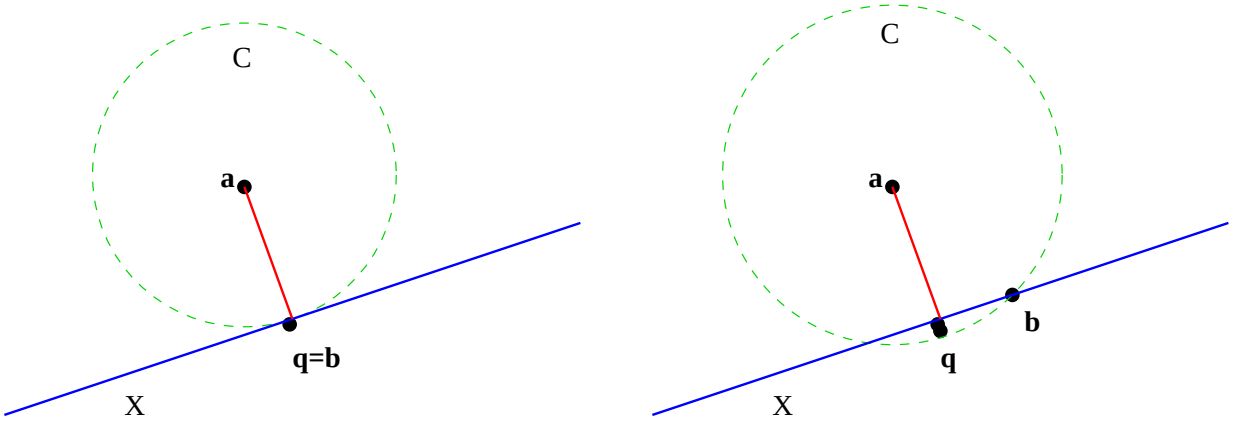


Figure 6.6: The line from $\mathbf{p}$ to $\text{Proj}(\mathbf{p}, X)$ is perpendicular to X.

- In two-dimensional graphics, moving an image in the picture plane.
- In computations involving solid objects, such as robotics or CAD/CAM, calculating the motion of a solid object through space.
- In graphics or computer vision, determining how an object moving through space appears in an image.

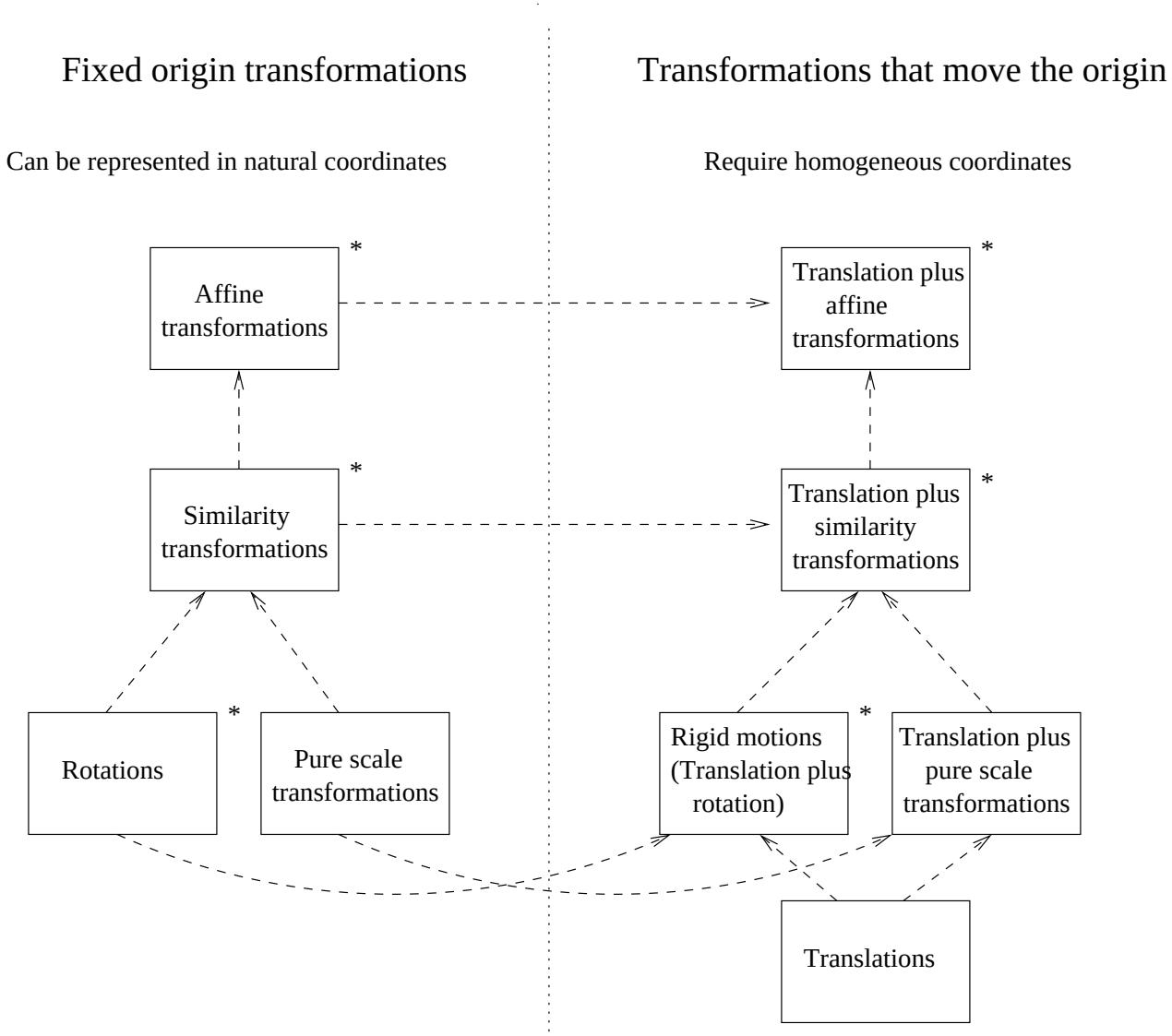
What linear algebra gives us is a language for characterizing the relation of one particular position of an object to another particular position. Such a relation is called a *geometric transformation.* We will not here be concerned with describing the continuous motion of an object over time, in which it moves through a whole range of positions; that requires calculus or analysis, and is beyond the scope of this book.

Geometrical transformations fall into categories, such as translations, rotations, rigid motions, and so on. The categories are organized in a hierarchy; for example, the category of rigid motions includes the category of translations.

The categories of geometric transformations that we will study here are (naturally) those that can be expressed by simple operations on coordinate vectors, particularly linear transformations. With many kinds of geometric transformations, doing this elegantly requires introducing a new method of representing points as numeric vectors. So far we have used the *natural* representation, in which a geometric point in two-space is represented by a two-dimensional vector and point in three-space is represented by a three-dimensional vector. In the new representation, called the *homogeneous* representation, a point in two-space is represented by a three-dimensional vector and a point in three-space is represented by a four-dimensional vector. The homogeneous representation will be introduced in section 6.4.3.

An important — indeed, a defining — characteristic of each category of geometric transformations is the class of *invariants* of the category; that is, geometric features or relations that are left unchanged by transformations in the category. For instance, a transformation Γ is a translation if and only if point subtraction $\mathbf{q} - \mathbf{p}$ is an invariant; that is, for all points $\mathbf{p}, \mathbf{q}$, $\Gamma(\mathbf{q}) - \Gamma(\mathbf{p}) = \mathbf{q} - \mathbf{p}$. A transformation Γ is in the class of rigid mappings with reflection if distance is an invariant; that is, if $d(\Gamma(\mathbf{p}), \Gamma(\mathbf{q})) = d(\mathbf{p}, \mathbf{q})$ for all points $\mathbf{p}, \mathbf{q}$.

Figure 6.7 shows the hierarchy of categories of transformations that we consider here.



A dashed arrow from category C to category D means that D includes C.
Any category C with an asterisk is actually two categories:

- C.1: The transformations in C excluding reflections.
- C.2: All transformations in C, including reflections.

Category C.2 includes C.1.

Figure 6.7: Hierarchy of categories of transformations

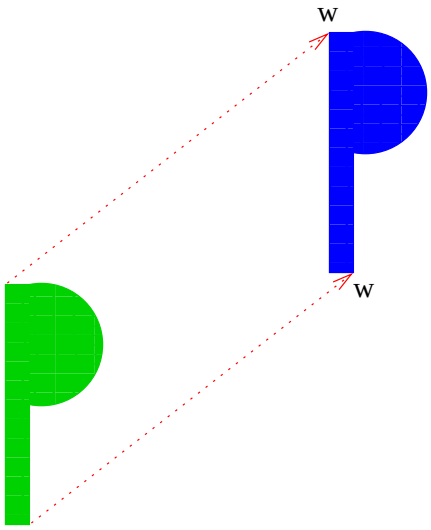


Figure 6.8: Translation

6.4.1 Translations

For any arrow $\vec{v}$, the *translation* by $\vec{v}$ is the function that moves every point in parallel by $\vec{v}$; that is, $\Gamma(\mathbf{p}) = \mathbf{p} + \vec{v}$ for every point $\mathbf{p}$. Thus, a translated figure is moved in the two-space or three-space changing only the position, keeping the shape and the orientation constant (figure 6.8).

The fundamental invariant of a translation is point subtraction; if Γ is a translation then $\Gamma(\mathbf{q}) - \Gamma(\mathbf{p}) = \mathbf{q} - \mathbf{p}$ for all points $\mathbf{p}, \mathbf{q}$. It follows as a consequence that distances, angles, and orientations are all invariants of a translation.

Translation is an simple but important category in computer graphics; moving a window or an image in a display is (usually) a pure translation.

In natural coordinates, the coordinates of the translation of point $\mathbf{p}$ by vector $\vec{v}$ are just the sum of the coordinates of $\mathbf{p}$ plus the coordinates of $\vec{v}$. Translations are easily composed and inverted. If $\mathbf{p}$ is translated first by $\vec{v}$ and then by $\vec{u}$, the result is the same as a single translation by $\vec{v} + \vec{u}$. The inverse of translating $\mathbf{p}$ by $\vec{v}$ is translating it by $-\vec{v}$.

6.4.2 Rotation around the origin

In two space, a rotation around the origin is carried out by drawing the figure on a piece of paper on a desk, sticking a thumbtack through the paper to the desk at the origin, and turning the paper while leaving the origin fixed. In three space, a rotation around the origin is carried out by taking a solid object, marking one point on the object as the origin, and then twisting the object in space while keeping the origin fixed in place. Mechanically, this can be done by attaching the object to a fixed frame using a ball joint, where the center of the joint is at the origin.

Rotations around the origin in two space

Let us start with the two-dimensional case, which is easier to visualize and to illustrate. Rotations can be characterized in terms of coordinate vectors as follows. We have a board, which is fixed,

and a paper attached by a thumbtack at the origin, which rotates; we want to know how points drawn on the paper move; and we will measure this motion using a fixed coordinate system drawn on the board. Put the paper in its starting position. On the paper draw the unit x and y arrows, $\vec{\vec{x}}$ and $\vec{\vec{y}}$, placing their tails at the origin. Draw a dot at any point $\mathbf{p}$ with coordinates $\langle a, b\rangle$. Thus $\mathbf{p} = \mathbf{o} + a\vec{\vec{x}} + b\vec{\vec{y}}$. Now rotate the paper. Let $\Gamma(\vec{\vec{x}})$, $\Gamma(\vec{\vec{y}})$ and $\Gamma(\mathbf{p})$ be the new positions of the arrows and the dots. Clearly the relations on the paper between $\mathbf{o}, \mathbf{p}, \vec{\vec{x}}$, and $\vec{\vec{y}}$ have not changed, so we have $\Gamma(\mathbf{p}) = \mathbf{o} + a\Gamma(\vec{\vec{x}}) + b\Gamma(\vec{\vec{y}})$. Let $\mathcal{C}$ be the fixed coordinate system attached to the board; and let $\vec{p} = \text{Coords}(\mathbf{p}, \mathcal{C})$, $\vec{p}^{\,'} = \text{Coords}(\Gamma(\mathbf{p}), \mathcal{C})$, $\vec{x}^{\,'} = \text{Coords}(\Gamma(\mathbf{x}), \mathcal{C})$, $\vec{y}^{\,'} = \text{Coords}(\Gamma(\mathbf{y}), \mathcal{C})$. Then we have $\vec{p}^{\,'} = a\vec{x}^{\,'} + b\vec{y}^{\,'}$.

Let R be the matrix whose columns are $\vec{x}^{\,'}$ and $\vec{y}^{\,'}$. Then we can write this equation as $\vec{p}^{\,'} = R\vec{p}$. In other words, the result of the rotation Γ corresponds to matrix multiplication by the matrix R.

For example, figure 6.9 shows a case where $\vec{p} = \langle 3.5, 2\rangle$, and Γ is a rotation by 30°. Then $\Gamma(\vec{\vec{x}}) = \langle \cos(30°), \sin(30°)\rangle = \langle .866, 0.5\rangle$ and $\Gamma(\vec{\vec{y}}) = \langle -\sin(30°), \cos(30°)\rangle = \langle -0.5, 8.66\rangle$ so

$$\Gamma(\mathbf{p}) = \begin{bmatrix} 0.866 & -0.5 \\ 0.5 & 0.866 \end{bmatrix} \cdot \begin{bmatrix} 3.5 \\ 2 \end{bmatrix} = \begin{bmatrix} 2.03 \\ 3.48 \end{bmatrix}$$

What can we say about the matrix R? One thing we can do is to calculate it. If Γ is a positive rotation by angle θ then, by trigonometry, the coordinates of $\Gamma(\vec{\vec{x}})$ are $\langle \cos(\theta), \sin(\theta)\rangle$ and the coordinates of $\Gamma(\vec{\vec{y}})$ are $\langle -\sin(\theta), \cos(\theta)\rangle$ so R is the matrix

$$R = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$$

But that is trigonometry, not linear algebra (hence the non-linear functions). From the standpoint of linear algebra, we can observe that, since we are not folding or bending the paper, the rotated arrows $\Gamma(\vec{\vec{x}})$ and $\Gamma(\vec{\vec{y}})$ still have length 1 and are still at right angles. Since the coordinates of these two arrows are the columns of R, that means that the columns of R have the following elegant properties:

- $R[:, i] \bullet R[:, i] = 1$.
- If $i \neq j$ then $R[:, i] \bullet R[:, j] = 0$.

Thus, R is an orthonormal matrix, so $R^T \cdot R = I$.

It is easy to show that, for any orthonormal matrix R and vectors $\vec{v}$ and $\vec{u}$, the length of $\vec{v}$ and the angle between $\vec{v}$ and $\vec{u}$ is invariant under multiplication by R. We can show both of these by showing that the dot product is invariant, as follows:

$$((R\vec{u}) \bullet (R\vec{v}) = (R\vec{u})^T R\vec{v} = \vec{u}^T R^T R\vec{u} = \vec{u}^T \vec{v} = \vec{u} \bullet \vec{v}$$

We have shown that any rotation around the origin corresponds to multiplication by an orthonormal matrix. Is the converse true? Unfortunately, not quite. Consider the matrix,

$$R = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

Then the product

$$R \cdot \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -x \\ y \end{bmatrix}$$

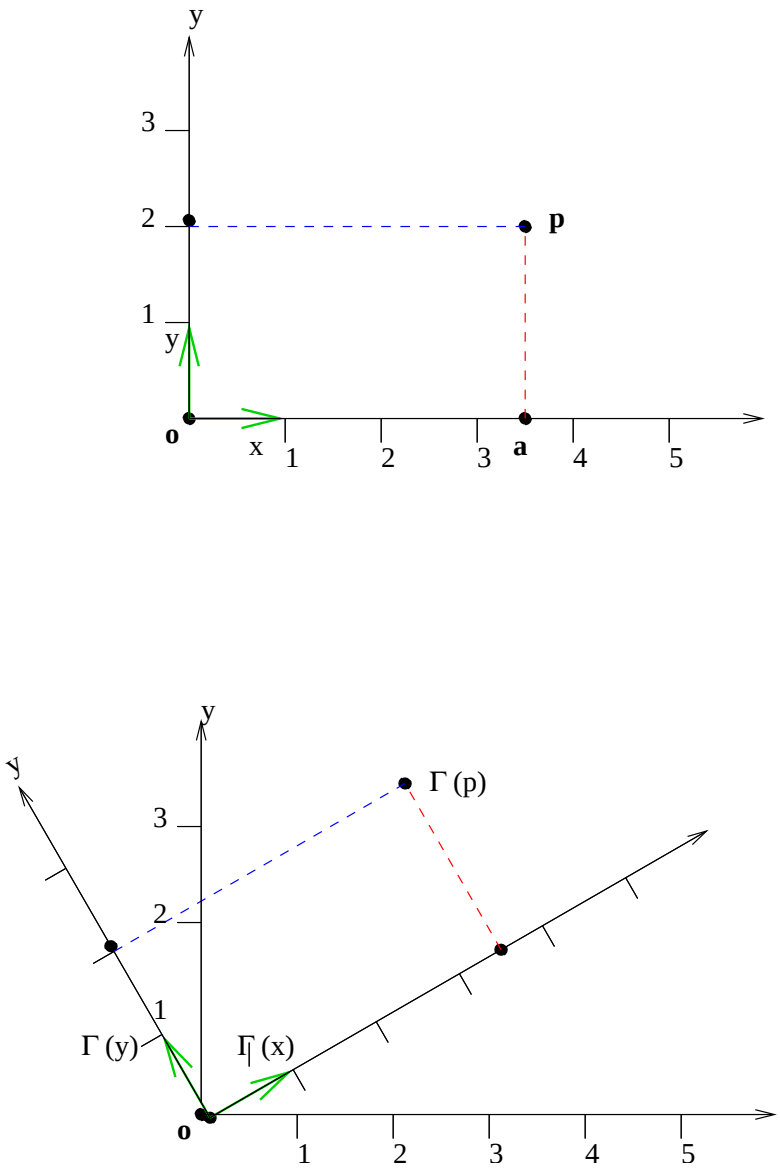


Figure 6.9: Rotation around the origin

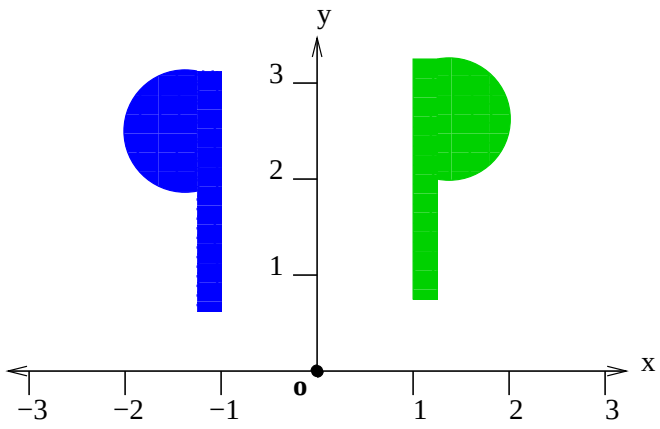


Figure 6.10: Reflection

The effect of multiplication by R on a "P"-like shape is shown in figure 6.10. The blue "P" is not a rotation of the green "P"; there is no way of turning the paper to make the green "P" line up with the blue "P". The only way is to hold up the paper to the mirror, or to draw the green P on thin paper and look at it through the paper from the other side. In short the blue "P" is a *reflection* of the green "P"; in this case, the reflection across the y-axis.

A reflection across a line through the origin also corresponds to an orthonormal matrix. Conversely, if R is an orthonormal matrix then multiplication by R carries out either a rotation around the origin or a reflection across a line through the origin.

Note that a reflection also changes the sign of angles between directions. For instance, the signed angle from $\vec{x}$ to $\vec{y}$ is 90° counterclockwise. The reflection matrix R maps $\vec{x}$ to $-\vec{x}$ and maps $\vec{y}$ to itself, and the signed angle from $-\vec{x}$ to $\vec{y}$ is −90° counterclockwise. However, since the dot product just gives the cosine of the angle, and $\cos(-\theta) = \cos(\theta)$, there is no way to detect this from the dot product.

How do you tell a matrix that carries out a reflection from a rotation? The solution is to use the *determinant*.[3] The determinant of a 2×2 matrix is given by the formula,

$$\text{Det}\left(\begin{bmatrix} a & b \\ c & d \end{bmatrix}\right) = ad - bc$$

For any orthonormal matrix R, either $\text{Det}(R) = 1$, in which case R is a rotation, or $\text{Det}(R) = -1$, in which case R is a reflection. We will discuss determinants further in section 6.4.7.

The invariants associated with rotations and reflections around the origin are:

- The position of the origin.
- The distance between any two points.
- The unsigned angle between any two directions.

If we exclude reflections, then the invariants associated purely with rotations include also the signed angle between any two directions.

[3]Determinants are, in general not extremely important for the kinds of applications we are considering in this book, so we are treating them at much less length than most linear algebra texts.

Rotations around the origin in three-space

The linear algebra associated with rotations around the origin in three-space is almost the same as in two-space; the trigonometry is considerably more difficult.

The argument above that proves that a rotation around the origin corresponds to multiplication by an orthonormal matrix works in three-dimensions in exactly the same way as in two dimensions. All we need to do it to add a third coordinate vector $\vec{\vec{z}}$. In particular: Let Γ be any rotation around the origin in three-space. Let $\mathbf{p}$ be any point. Let $\mathcal{C}$ be a coordinate system with origin $\mathbf{o}$ and unit direction arrows $\vec{\vec{x}}, \vec{\vec{y}}, \vec{\vec{z}}$. Let $\vec{p} = \text{Coords}(\mathbf{p}, \mathcal{C})$, $\vec{p}^{\,\prime} = \text{Coords}(\Gamma(\mathbf{p}), \mathcal{C})$, $\vec{x}^{\,\prime} = \text{Coords}(\Gamma(\mathbf{x}), \mathcal{C})$, $\vec{y}^{\,\prime} = \text{Coords}(\Gamma(\mathbf{y}), \mathcal{C})$, $\vec{z}^{\,\prime} = \text{Coords}(\Gamma(\mathbf{z}), \mathcal{C})$. Let R be the 3×3 matrix whose columns are $\vec{x}^{\,\prime}$, $\vec{y}^{\,\prime}$, and $\vec{z}^{\,\prime}$.

Then:

- $\vec{p}^{\,\prime} = R \cdot \vec{p}$;
- R is an orthonormal matrix; that is, $R^T \cdot R = I$.

Conversely, if R is an orthonormal matrix, then multiplication by R corresponds either to a rotation around the origin or to reflection across a plane through the origin. In three-space, a reflection transforms a left-hand glove into a right-hand glove and vice versa, or a left-hand screw into a right-hand screw; luckily for the manufacturers of gloves and unluckily for those of us who wear and lose gloves, there is no way to achieve this using rotation. An orthonormal matrix R is rotation without reflection if its determinant is 1; it is a reflection if its determinant is -1. The determinant of a 3×3 matrix will be defined in section 6.4.7.

The trigonometry of three-space rotations, however, is much more complicated than the trigonometry of two-space rotations. Just as a rotation around the origin in two-space can be represented in terms of a single angle θ, a rotation around the origin in three-space can be represented in terms of three angles θ, ϕ, ψ. However:

- Whereas in two-space, there is only one reasonable way to represent a rotation as an angle, in three-space there are many different ways; in fact there are several different ways that are used in practice.
- Any method of representing three-space rotations in terms of three angles necessarily suffers from "topological singularities" where the representation becomes severely awkward.
- In two-space, the same angle representation can be used for both directions and rotations. In three-space, directions are represented by *two* angles (e.g. latitude and longitude), whereas rotations are represented by *three* angles.
- In two-space, the composition of a rotation by θ followed by a rotation by ϕ is just a rotation by $(\theta + \phi) \bmod 2\pi$. No representation of three-space rotations in terms of angles has anything like so simple a rule for composition; in fact to compute a composition, it is generally easiest to convert to matrix notation, do matrix multiplication, and convert back.

We will discuss one particular simple case of three-dimensional rotations in section 7.1.3.

6.4.3 Rigid motions and the homogeneous representation

At this point, we know how to calculate the result of translating a figure and of rotating a figure around the origin. But suppose that we want to move an object freely around space, combining

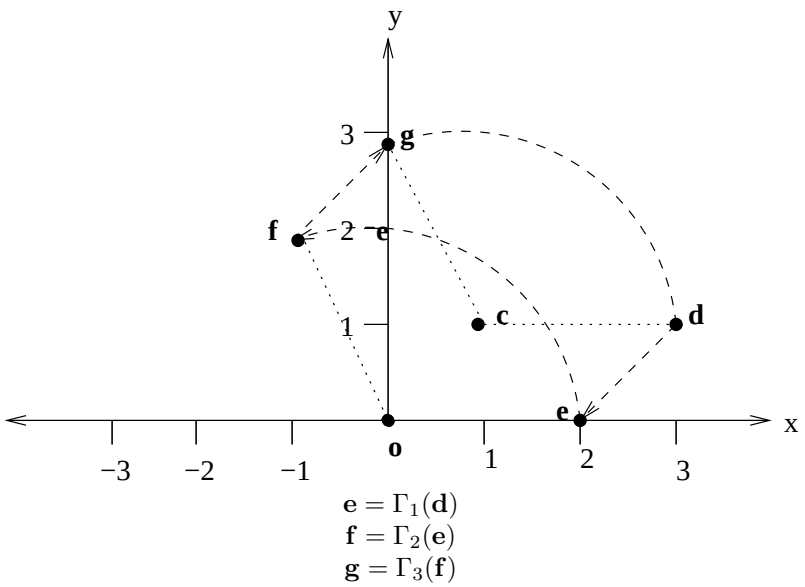


Figure 6.11: Rotation around a point that is not the origin

rotations and translations as the spirit moves us. Or suppose that we want carry out a rotation around some point that is not the origin? Such a transformation is called a *rigid motion.* Again, there is a distinction between rigid transformations that are not reflections, which actually can be physically carried out by turning the object around, and those that are reflections, which cannot be achieved by any kind of turning. A rigid motion preserves distances and angles.

One way to do combine translations and rotations is just to carry out a sequence of vector additions and matrix multiplications on the natural coordinates, One can also perform rotations around points other than the origin in this way. For instance (figure 6.11), let **c** and **d** be the points with coordinates $\langle 1, 1\rangle$ and $\langle 3, 1\rangle$, and suppose that you want to compute the location of **d** after performing a rotation of 120° around **c**. This can be done as a sequence of three transformation

- Γ_1 is a translation by $\mathbf{o} - \mathbf{c}$, computed by adding the vector $\langle -1, -1\rangle$. Thus $\Gamma_1(\mathbf{c}) = \langle 0, 0\rangle$; $\Gamma_1(\mathbf{d}) = \langle 2, 0\rangle$.
- Γ_2 is a rotation around **o** by 120°, computed by multiplying by the matrix

$$\begin{bmatrix} -0.5 & 0.866 \\ -0.866 & -0.5 \end{bmatrix}$$

  Thus $\Gamma_2(\Gamma_1(\mathbf{c})) = \langle 0, 0\rangle$; $\Gamma_2(\Gamma_1(\mathbf{d})) = \langle -1.0, 1.732\rangle$.
- Γ_3 is a translation by $\mathbf{c} - \mathbf{o}$, computed by adding the vector $\langle 1, 1\rangle$. Thus $\Gamma_3(\Gamma_2(\Gamma_1(\mathbf{c}))) = \langle 1, 1\rangle$; $\Gamma_3(\Gamma_2(\Gamma_1(\mathbf{d}))) = \langle 0, 1.732\rangle$.

The composition $\Gamma_3 \circ \Gamma_2 \circ \Gamma_1$ is the desired transformation.

If you are doing a one-time calculation, this may actually be the easiest approach, but it becomes awkward if you want to do many such calculations, particularly if you want to compose rigid motions.

There is really no way around this using natural coordinates. Obviously, rotation does not correspond to any kind of vector addition. Almost equally obviously, translation does not correspond to any

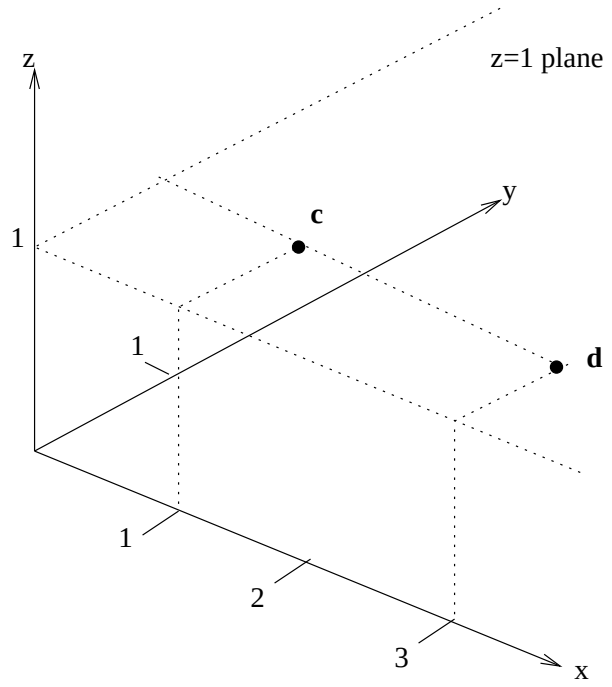


Figure 6.12: Homogeneous Coordinates

kind of matrix multiplication, because translation moves all points and matrix multiplication leaves the zero vector unchanged.

The solution is to use a different coordinate representation, called *homogeneous coordinates.*[4] In homogeneous coordinates, as in natural coordinates, a coordinate system is still defined in terms of an origin $\mathbf{o}$ and two or three coordinate arrows $\vec{x}$, $\vec{y}$ and in three-space $\vec{z}$. However, a point in two-space is represented by a three-dimensional numeric vector; the first two coordinates are the natural coordinates, and the third coordinate is always 1. A point in three-space is represented by a four-dimensional numeric vector; the first three coordinates are the natural coordinates, and the fourth coordinate is always 1. Arrows in two-space and three-space are likewise represented using three and four dimensional vectors; the first two/three coordinates are the natural coordinates, and the last coordinate is 0.

We will denote homogeneous coordinates of point $\mathbf{p}$ or arrow $\vec{v}$ with respect to coordinate system $\mathcal{C}$ as $\mathrm{Hc}(\mathbf{p},\mathcal{C})$ and $\mathrm{Hc}(\vec{v},\mathcal{C})$. For example, in figure 6.11, $\mathrm{Hc}(\mathbf{c},\mathcal{C}) = \langle 1,1,1\rangle$; $\mathrm{Hc}(\mathbf{d},\mathcal{C}) = \langle 3,1,1\rangle$; and $\mathrm{Hc}(\mathbf{d}-\mathbf{c},\mathcal{C}) = \langle 2,0,0\rangle$. We will often omit the argument $\mathcal{C}$, in cases where the coordinate system is fixed.

The basic arithmetical operations on points and arrows in terms of coordinates still work as before; $\mathrm{Hc}(\mathbf{p}+\vec{v}) = \mathrm{Hc}(\mathbf{p}) + \mathrm{Hc}(\vec{v})$ and so on. Likewise, the length of $\vec{v}$ is equal to $|\,\mathrm{Hc}(\vec{v})|$, and the angle θ between $\vec{u}$ and $\vec{v}$ satisfies

$$\cos(\theta) = \frac{\mathrm{Hc}(\vec{u}) \bullet \mathrm{Hc}(\vec{v})}{|\,\mathrm{Hc}(\vec{u})| \cdot \mathrm{Hc}(\vec{v})|}$$

[4]Strictly speaking, the representation we discuss here is known as *normalized homogeneous coordinates.* There is a more general version of homogeneous coordinates, in which a point with natural coordinates $\langle a,b\rangle$ is represented by a vector $\langle ra,rb,r\rangle$ for any $r \neq 0$.

We can visualize this as follows, at least in the case of the three-dimensional representation of two-space.[5] We are representing geometric two-space as the plane $z = 1$ in three-dimensional vector space (figure 6.12). The homogeneous coordinates of a point $\mathbf{p}$ relative to the plane are the natural coordinates of the vector $\mathbf{p} - \mathbf{o}_3$ where $\mathbf{o}_3$ is the origin of the embedding 3-space. An two-space arrow $\vec{\vec{v}}$ is represented by the corresponding point in the plane $z = 0$. (Note also that this eliminates the confusion, discussed earlier, between visualizing points and visualizing arrows.)

The advantage of using homogeneous coordinates is that now both rotation and translation correspond to multiplying the coordinate vector by a transformation matrix, so the composition of two transformation is just the matrix product of the corresponding transformation matrices. Specifically: A translation by arrow $\vec{\vec{v}}$ which has natural coordinates $\vec{v}$ corresponds to multiplication of the homogeneous coordinates by the matrix

$$\left[\begin{array}{c|c} I & \vec{v} \\ \hline \vec{0}^T & 1 \end{array}\right]$$

If rotation Γ around the origin is represented in natural coordinates as matrix R, then it is represented in homogeneous coordinates by matrix

$$\left[\begin{array}{c|c} R & \vec{0} \\ \hline \vec{0}^T & 1 \end{array}\right]$$

The notation above, with horizontal and vertical lines, describes the division of the matrix into subrectangles. For instance,

$$\text{if } \vec{v} = \begin{bmatrix} 5 \\ 6 \end{bmatrix} \text{ then } \left[\begin{array}{c|c} I & \vec{v} \\ \hline \vec{0}^T & 1 \end{array}\right] \text{ denotes the matrix } \begin{bmatrix} 1 & 0 & 5 \\ 0 & 1 & 6 \\ 0 & 0 & 1 \end{bmatrix}$$

Applying this to the above example of rotating point $\mathbf{d}$ around point $\mathbf{c}$, again we consider the overall transformation Γ as the composition of the three transformations $\Gamma_3 \circ \Gamma_2 \circ \Gamma_1$, but since all these transformations are now matrix multiplication, their composition corresponds to the product of the matrices. Specifically,

$$\Gamma_1 = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{bmatrix} \qquad \Gamma_2 = \begin{bmatrix} 0.866 & -0.5 & 0 \\ 0.5 & 0.866 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \Gamma_3 = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\text{so } \Gamma = \Gamma_3 \cdot \Gamma_2 \cdot \Gamma_1 = \begin{bmatrix} 0.866 & -0.5 & 6.34 \\ 0.5 & 0.866 & -0.366 \\ 0 & 0 & 1 \end{bmatrix} \text{ and } \Gamma \cdot \mathbf{d} = \begin{bmatrix} 2.732 \\ 2 \\ 1 \end{bmatrix}$$

In general, for any rigid transformation Γ, the corresponding matrix in homogeneous coordinates has the form

$$\left[\begin{array}{c|c} R & \vec{v} \\ \hline \vec{0}^T & 1 \end{array}\right]$$

[5] This also works in principle for the four-dimensional representation of three-space, but most people find that harder to visualize.

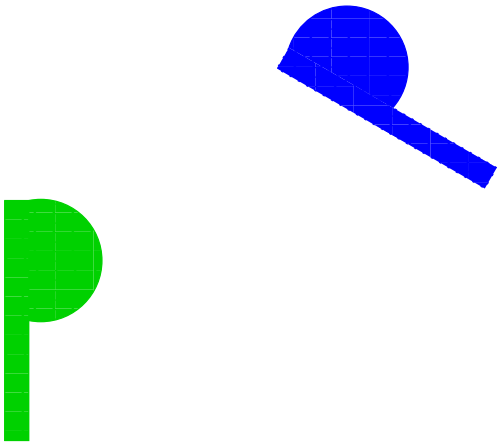


Figure 6.13: Rigid motion

where R is an orthonormal Since this is equal to

$$\left[\begin{array}{c|c} I & \vec{v} \\ \hline \vec{0}^T & 1 \end{array}\right] \cdot \left[\begin{array}{c|c} R & \vec{0} \\ \hline \vec{0}^T & 1 \end{array}\right]$$

this expresses Γ as the composition of the rotation around the origin described by R in natural coordinates, followed by a translation by $\vec{v}$.

Conversely, if R is an orthonormal matrix, and $\vec{v}$ is a vector, then the matrix

$$A = \left[\begin{array}{c|c} R & \vec{v} \\ \hline \vec{0}^T & 1 \end{array}\right]$$

corresponds to a rigid motion in homogeneous coordinates. A is not a reflection if $\mathrm{Det}(R) = 1$; A is a reflection if $\mathrm{Det}(R) = -1$. (As we shall see below, $\mathrm{Det}(A) = \mathrm{Det}(R)$.)

The invariants of a rigid motion are:

- The distance between two points and the length of an arrow.
- The angle between two arrows.

6.4.4 Similarity transformations

A *similarity* or *scale* transformation expands or contracts everything by a constant factor in all directions (figure 6.14). This is important in imaging applications; in graphics, it is often necessary to expand or contract an image without otherwise distorting it; in vision, the image of an object expands or contracts as the distance from the eye to the object increases or decreases. It is not very important in physical applications, since physical objects rarely expand and contract uniformly.

The simplest form of scale transformation is change of scale without rotation, reflection, or translation. This corresponds to a simple scalar multiplication of natural coordinates:

$$\mathrm{Coords}(\Gamma(\mathbf{p}), \mathcal{C}) = c \cdot \mathrm{Coords}(\mathbf{p}, \mathcal{C})$$

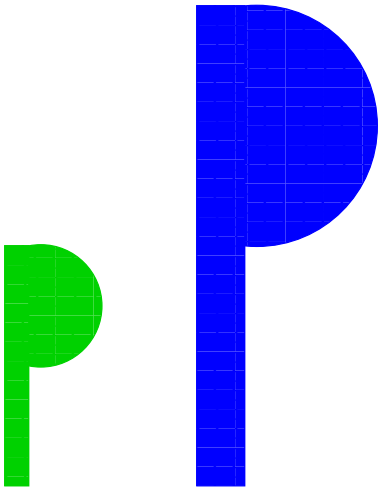


Figure 6.14: Scale Transformation

where $c > 0$.

In homogeneous coordinates, this corresponds to multiplication by the matrix

$$\left[\begin{array}{c|c} c \cdot I & \vec{0} \\ \hline \vec{0}^T & 1 \end{array}\right] \text{ where } c > 0.$$

For example, if $\mathbf{p}$ is the point $\langle 3, 5\rangle$ and Γ is a scale expansion by a factor of 2. Then the natural coordinates of $\Gamma(\mathbf{p})$ are $2 \cdot \langle 3, 5\rangle = \langle 6, 10\rangle$. The homogeneous coordinates of $\Gamma(\mathbf{p})$ are

$$\begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 3 \\ 5 \\ 1 \end{bmatrix} = \begin{bmatrix} 6 \\ 10 \\ 1 \end{bmatrix}$$

The invariants of a pure scale transformation of this kind are position of the origin; directions of arrows; angles between arrows; and ratios between distances (that is, for any points $\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{s}$ $d(\mathbf{p}, \mathbf{q})/d(\mathbf{r}, \mathbf{s})$ is unchanged).

The most general form of scale transformation combines it with a rotation, reflection, and/or translation. In homogeneous coordinates, this corresponds to multiplication by a matrix of the form

$$\left[\begin{array}{c|c} c \cdot R & \vec{v} \\ \hline \vec{0}^T & 1 \end{array}\right]$$

where $c \neq 0$ and R is a orthonormal matrix.

Conversely, a matrix M corresponds to a general scale transformation if the following conditions hold. Let A be the upper left hand corner of such a matrix (that is, all but the last row and column). Then

- The last row of M has the form $\langle 0...0, 1\rangle$.
- $A^T A$ is a diagonal matrix with the same value (c^2) all along the main diagonal and 0 elsewhere.

The transformation is not a reflection if $\mathrm{Det}(A) > 0$. It is a reflection if $\mathrm{Det}(A) < 0$.

The invariants of a general scale transformation are the angles between arrows and ratios of distances.

6.4.5 Affine transformations

For the final class of transformations, it is easiest to go in the opposite direction, from matrices to geometry. Let M be any matrix of the form

$$M = \left[\begin{array}{c|c} A & \vec{v} \\ \hline \vec{0}^T & 1 \end{array}\right]$$

Then multiplication by M transforms one vector of homogeneous coordinates (i.e. vector with final component 1) to another. What is the geometric significance of this operation?

To answer that, it is easiest to consider the case where $\vec{v} = \vec{0}$, so that the origin remains fixed. In this case, the transformation can also be viewed as matrix multiplication of the natural coordinates of a point by the matrix A; that is

$$\mathrm{Coords}(\Gamma(\mathbf{p}), \mathcal{C}) = A \cdot \mathrm{Coords}(\mathbf{p}, \mathcal{C})$$

In two-space, let $\vec{\vec{x}}$ and $\vec{\vec{y}}$ be the x and y coordinate arrows. Let $\mathbf{p}$ be a point with coordinates $\langle a, b\rangle$. Then we have

$$\mathrm{Coords}(\Gamma(\vec{\vec{x}}), \mathcal{C}) = A \left[\begin{array}{c} 1 \\ 0 \end{array}\right] = A[:, 1] \text{ and } \mathrm{Coords}(\Gamma(\vec{\vec{y}}), \mathcal{C}) = A \left[\begin{array}{c} 0 \\ 1 \end{array}\right] = A[:, 2]$$

so

$$\mathrm{Coords}(\Gamma(\mathbf{p}), \mathcal{C}) = A \left[\begin{array}{c} a \\ b \end{array}\right] = aA[:, 1] + bA[:, 2] = a \cdot \mathrm{Coords}(\Gamma(\vec{\vec{x}}), \mathcal{C}) + b \cdot \mathrm{Coords}(\Gamma(\vec{\vec{y}}), \mathcal{C})$$

In other words, what Γ does is to map the coordinate directions $\vec{\vec{x}}$ and $\vec{\vec{y}}$ to two other vectors $\Gamma(\vec{\vec{x}}), \Gamma(\vec{\vec{y}})$, and then maps any point with coordinates $\langle a, b\rangle$ to the point $a\Gamma(\vec{\vec{x}}) + b\Gamma(\vec{\vec{y}})$. The result is in general a rotation and a skewing of the figure. For instance figure 6.15 shows the affine transformation corresponding to multiplication by the transformation

$$M = \left[\begin{array}{cc} 1/4 & -1/2 \\ 1/2 & 1 \end{array}\right]$$

Here $\Gamma(\vec{x}) = \langle 1/4, 1/2\rangle$ and $\Gamma(\vec{y}) = \langle -1/2, 1\rangle$.

If $\Gamma(\vec{\vec{x}}), \Gamma(\vec{\vec{y}})$ are not parallel, then rank(A)=2, and Γ is a bijection of the plane to itself. If $\Gamma(\vec{\vec{x}})$ and $\Gamma(\vec{\vec{y}})$ are parallel, then rank(A)=1, and any point $\mathbf{p}$ is mapped onto a point on the line $\{\mathbf{o} + t\Gamma(\vec{\vec{x}}) | t \in \mathbb{R}\}$; that is, the plane is collapsed down into a line. If $\Gamma(\vec{\vec{x}}) = \Gamma(\vec{\vec{y}}) = \vec{0}$, then Rank$(A)$=0 and Γ collapses the plane down to a point. A transformation that maps the plane to a line or a point is said to be *degenerate*; a transformation that maps the plane to the plane is *invertable*.

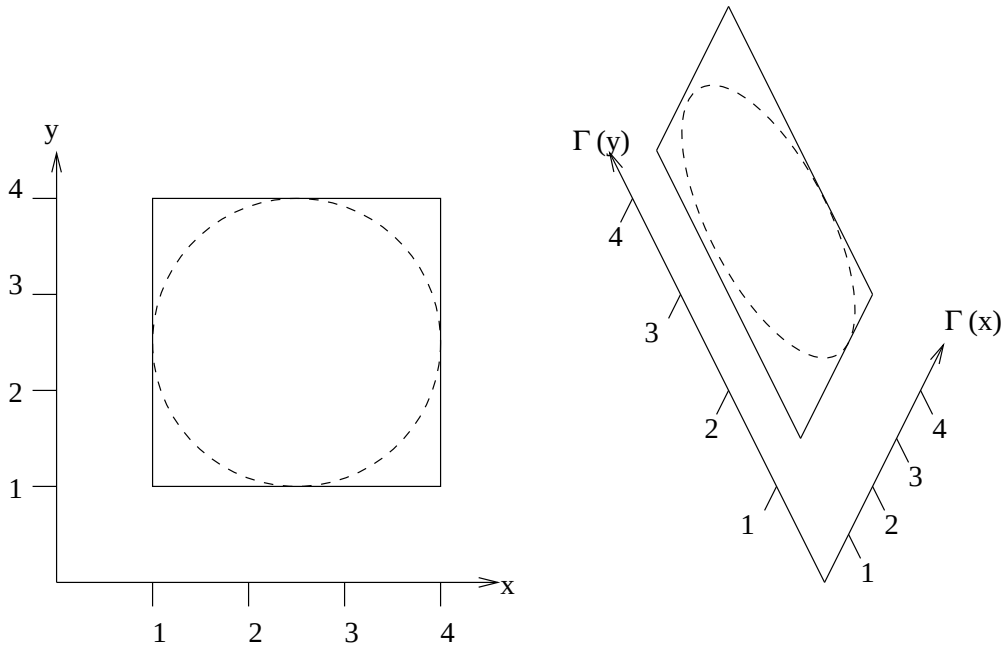


Figure 6.15: Affine Transformation

The general affine transformation corresponds to multiplication of homogeneous coordinates by a matrix M of the form

$$\left[\begin{array}{c|c} A & \vec{v} \\ \hline \vec{0}^T & 1 \end{array}\right]$$

This is the composition of an affine transformation A around the origin, followed by a translation of $\vec{v}$.

Affine transformations in three-space are similar. Let $\vec{x}, \vec{y}, \vec{z}$ be the coordinate directions and let point $\mathbf{p} = a\vec{x} + b\vec{y} + c\vec{z}$. Then an affine transformation maps $\mathbf{p}$ to the point $\Gamma(\mathbf{p}) = \vec{v} + a\Gamma(\vec{x}) + b\Gamma(\vec{y}) + c\Gamma(\vec{z})$, where $\vec{v}$ is the translation part of the mapping, independent of $\mathbf{p}$. If Rank(A)=3, then Γ maps the plane to itself; that is, Γ is invertable. If Rank(A)=2, 1, or 0 then Γ collapses the plane to a plane, a line, or a point respectively; that is, Γ is degenerate.

The case where $\Gamma(\vec{x}) = a\vec{x}, \Gamma(\vec{y}) = b\vec{y}$ corresponds to a change in the aspect ratio, an operation available in most image editors. Otherwise, the primary application for geometric affine transformation is in images of objects rotating in three space, as described below.

The fundamental invariant of an affine transformation Γ is identity of point subtraction; that is, if $\mathbf{b} - \mathbf{a} = \mathbf{d} - \mathbf{c}$ then $\Gamma(\mathbf{b}) - \Gamma(\mathbf{a}) = \Gamma(\mathbf{d}) - \Gamma(\mathbf{c})$. It follows from this that Γ is defined over arrows and that addition of arrows to one another and to points and scalar multiplication of arrows are likewise invariants; that is,

$\Gamma(\mathbf{a} + \vec{u}) = \Gamma(\mathbf{a}) + \Gamma(\vec{u})$.
$\Gamma(\vec{u} + \vec{v}) = \Gamma(\vec{u}) + \Gamma(\vec{v})$.
$\Gamma(c \cdot \vec{u}) = c \cdot \Gamma(\vec{u})$.

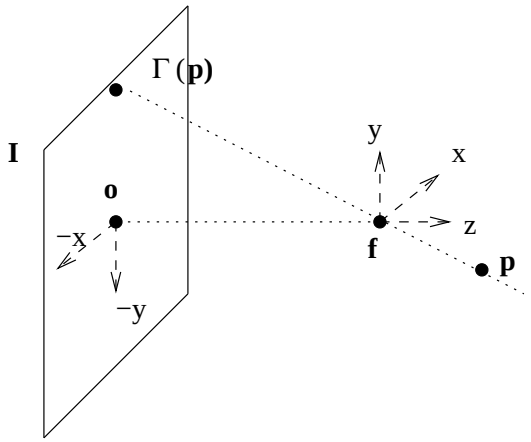


Figure 6.16: Projection onto an image plane

6.4.6 Image of a distant object

One application of linear transformations is to describe the changing image of a distant object moving in space.

In image formation, there is a lens with focal point **f** which projects an image onto a image plane **I** (figure 6.16). Any point in space **p** is projected onto a point $\Gamma(\mathbf{p})$, which is the intersection of the line **pf** with the plane **I**. To describe this, we will use two coordinate systems. Let **o** be the projection of **f** onto **I**. In the coordinate system $\mathcal{C}$ for three-space, the origin will be the focus **f**, the unit distance will be $\mathrm{d}(\mathbf{f},\mathbf{o})$, the z-axis $\vec{z} = \mathbf{o} - \mathbf{f}$ (note that this is perpendicular to **I**) and the other two axes $\vec{x}$ and $\vec{y}$ will be two other orthogonal vectors. Thus in coordinate system $\mathcal{C}$, I is the plane $z = -1$. In the coordinate system $\mathcal{B}$ for **I**, the origin **o** is the projection of **f** onto **I**, and the two coordinate axes are $-\vec{x}$ and $-\vec{y}$. Then for any point **p** in three space, if $\mathrm{Coords}(\mathbf{p},\mathcal{C}) = \langle x, y, z\rangle$ then $\mathrm{Coords}(\Gamma(\mathbf{p}),\mathcal{B}) = \langle x/z, y/z\rangle$. Note that for any fixed z this is linear in x and y but it is not linear in z.

Now, suppose we have a planar piece of lucite **P** that we can move around in space and we have drawn a region Q on **P**. We are interested in how the image of Q in **I** changes as we move **P**. In some important cases, this is a linear transformation or nearly so.

Case 1: Rigid motion. Suppose that **P** is moved by a translation $\vec{v}$ that is parallel to **I**. Then Then the image of Q undergoes a rigid motion with rotation R and translation $\vec{v}/z_0$.

(This may seem counter-intuitive; surely if you move **P** very far up or down, then the image of Q becomes small and foreshortened? That is because you are thinking of the case where you turn your eye or your head to keep Q in sight. If you are projecting onto a plane **I** which you keep constant, then this doesn't happen, because the projection is likewise far from the point **o**. This is only an adequate model of ocular vision in the case where Q remains quite close to a fixed line of sight.)

Case 2: Scale transformation. Suppose **P** is kept parallel to **I**, **P** is translated by arrow $\vec{v}$ which is parallel to $\vec{z}$ and the z-coordinate of P move from z_0 to $z_1 = z_0 + \vec{v} \bullet \vec{z}$. Then a point **p** in **P** moves from coordinates $\langle x, y, z_0\rangle$ to coordinates $\langle x, y, z_1\rangle$, so $\Gamma(\mathbf{p})$ moves from $\langle x/z_0, y/z_0\rangle$ to $\langle x/z_1, y/z_1\rangle$. That is, the image undergoes a scale transformation around the origin by a factor of z_0/z_1.

Case 3: Affine transformation. Let **P** be at any plane in space. Let **q** be point in the region Q.

Let $\vec{\vec{u}}$ and $\vec{\vec{v}}$ be two orthogonal unit arrows parallel to $\mathbf{P}$. Let z_0 be the z-coordinate of some point in Q; and assume that the diameter of Q is small as compared to z_0. Let $\mathbf{p}$ be a point in region Q whose coordinate in $\mathcal{D}$ are $\langle a, b\rangle$; thus $\mathbf{p} = \mathbf{q} + a\vec{\vec{u}} + b\vec{\vec{v}}$, where a and b are small as compared to z_0.

The coordinate vector of $\Gamma(\mathbf{p})$ in $\mathcal{B}$,

$$\text{Coords}(\Gamma(\mathbf{p}), \mathcal{B}) = \langle \frac{\vec{q}[x] + a\vec{u}[x] + b\vec{v}[x]}{\vec{p}_[z]}, \frac{\vec{q}[y] + a\vec{u}[x] + b\vec{v}[x]}{\vec{p}_[z]} \rangle$$

However, since $\vec{q}[z] - (a+b) \leq \vec{p}[z] \leq \vec{q}[z] + a + b$,
$\vec{q}[z] - (a+b) = z_0(1 - (a+b)/z_0)$, and
$\vec{q}[z] + (a+b) = z_0(1 + (a+b)/z_0)$,
we have $1/\vec{p}[z] \approx 1/z_0$. So

$$\text{Coords}(\Gamma(\mathbf{p}), \mathcal{B}) \approx \langle \frac{\vec{q}[x]}{z_0} + \frac{a\vec{u}[x] + b\vec{v}[x]}{z_0}, \frac{\vec{q}[y] + a\vec{u}[x] + b\vec{v}[x]}{z_0} \rangle = \begin{bmatrix} \vec{q}[x]/z_0 \\ \vec{q}[y]/z_0 \end{bmatrix} + \begin{bmatrix} \vec{u}[x]/z_0 & \vec{v}[x]/z_0 \\ \vec{u}[y]/z_0 & \vec{v}[y]/z_0 \end{bmatrix} \cdot \begin{bmatrix} a \\ b \end{bmatrix}$$

Thus the restriction of Γ to the region Q is approximately an affine transformation. It is easy to show that, if $\mathbf{P}$ is not perpendicular to $\mathbf{I}$, then there is an inverse Δ mapping $\Gamma(Q)$ to Q which is also an affine transformation.

Now, suppose that Q has image $\Gamma(Q)$, and Q undergoes a rigid transformation Φ, still satisfying the condition that the distance from Q to $\mathbf{I}$ is much greater than the diameter of Q. Then the image of the new position of Q is $\Gamma(\Phi(Q))$. Let W be the first image and Y be the second image; then we have $Y = \Gamma(\Phi(\Delta(W)))$. But then W and Y are related by the composition $\Gamma \circ \Phi \circ \Delta$; since all these are approximately affine transformations, their composition is also approximately an affine transformation. In short, two images of a moving planar figure are related by a transformation that is approximately an affine transformation, as long as the distance from the figure to the image plane is always much greater than the diameter of the figure.

Reflections in this scenario correspond to flipping the plane $\mathbf{P}$ around so that the eye is now looking at the back rather than the front. (This is why we imagined the figure as being drawn on lucite.)

One might ask, "Suppose we want to move a planar figure around in space freely, without restrictive assumptions, and we want an exact description of how the image changes, not an approximation?" The transformations involved then are *projective* transformations. Projective geometry is in many ways more interesting than affine geometry; however, as the transformation is non-linear, it is beyond the scope of this book.

6.4.7 Determinants

We defined above the *determinant* of a 2×2 matrix, and we alluded to the determinants of other matrices. The determinant function is very important in more advanced study of linear algebra; however, in the kinds of applications discussed in this book, it is not critical and rarely computed. In this section, we will briefly define the determinant of an $n \times n$ matrix and enumerate some of its properties, without proof or discussion.

To define the determinant of an $n \times n$ matrix we need the notion of the *minor* to an element of a matrix. If A is an $n \times n$ matrix and i and j are indices between 1 and n, then the minor to $A[i, j]$, denoted $C^{i,j}$, is the $(n-1) \times (n-1)$ matrix consisting of all the rows of A except the ith and all the columns of A except the jth.

We can now define the determinant recursively as follows:

- If A is the 1×1 matrix $[a]$ then $\text{Det}(A) = a$.

- If A is an $n \times n$ matrix for $n > 1$, let i be any index between 1 and n. Then

$$\mathrm{Det}(A) = \sum_{j=1}^{n} (-1)^{i+j} A[i,j] \cdot \mathrm{Det}(C^{i,j})$$

That is, one goes across the ith row, multiply $A[i,j]$ by the determinant of its minor, and add these products up, alternating signs at each step. The answer at the end is the same whatever row you choose.

Alternatively one can carry out the same operation, going down the jth column.

$$\mathrm{Det}(A) = \sum_{i=1}^{n} (-1)^{i+j} A[i,j] \cdot \mathrm{Det}(C^{i,j})$$

Again, you get the same answer, whichever column you choose.

Example: Let

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 0 & -1 \\ -3 & -2 & -4 \end{bmatrix}$$

Then, multiplying across the first row,

$$\mathrm{Det}(A) = 1 \cdot \mathrm{Det}(\begin{bmatrix} 0 & -1 \\ -2 & -4 \end{bmatrix}) - 2 \cdot \mathrm{Det}(\begin{bmatrix} 4 & -1 \\ -3 & -4 \end{bmatrix}) + 3 \cdot \mathrm{Det}(\begin{bmatrix} 4 & 0 \\ -3 & -2 \end{bmatrix}) =$$

$$1 \cdot ((0 \cdot -4) - (-2 \cdot -1)) - 2 \cdot ((4 \cdot -4) - (-1 \cdot -3)) + 3 \cdot ((4 \cdot -2) - (0 \cdot -3)) = (1 \cdot -2) - (2 \cdot -19) + (3 \cdot -8) = 12$$

Multiplying down the second column

$$\mathrm{Det}(A) = -2 \cdot \mathrm{Det}(\begin{bmatrix} 4 & -1 \\ -3 & -4 \end{bmatrix}) + 0 \cdot \mathrm{Det}(\begin{bmatrix} 1 & 3 \\ -3 & -4 \end{bmatrix}) - -2 \cdot \mathrm{Det}(\begin{bmatrix} 1 & 3 \\ 4 & -1 \end{bmatrix}) =$$

$$-2 \cdot ((4 \cdot -4) - (-3 \cdot -1)) + 0 - 2 \cdot ((1 \cdot -1) - (3 \cdot 4)) = (-2 \cdot -19) + (-2 \cdot -13) = 12$$

This formula is elegant, but it leads to a $O(n!)$ time algorithm. A more efficient algorithm uses row-echelon reduction. To compute $\mathrm{Det}(A)$ more efficiently, carry out the row-echelon reduction of A, adding the following steps:

1. At the start, set variable $D \leftarrow 1$.
2. Whenever you divide a row by a constant, $A[i,:] \leftarrow A[i,:]/c$, set $D \leftarrow c \cdot D$.
3. Whenever you swap two rows, set $D \leftarrow -D$.
4. Return D times the product of the elements in the main diagonal.

Note that D is not changed when the row echelon operation $A[j,:] \leftarrow A[j,:] - cA[i,:]$ is executed.

The following properties of the determinant should be noted: Let A be a $n \times n$ matrix, and let Γ be the transformation corresponding to multiplication by A.

- A is a singular matrix if and only if $\mathrm{Det}(A) = 0$.
- If $\mathrm{Det}(A) < 0$, then Γ is a reflection. If $\mathrm{Det}(A) > 0$ then Γ is not a reflection.

- If $n = 2$ and R is a region in two-space, then $\text{area}(\Gamma(R)) = |\operatorname{Det}(A)| \cdot \text{area}(R)$. If $n \geq 3$ and R is a region in three-space, then $\text{volume}(\Gamma(R)) = |\operatorname{Det}(A)| \cdot \text{volume}(R)$. The corresponding formula holds for $n > 3$ where "volume" is interpreted as n-dimensional volume. These formulas hold whether natural or homogeneous coordinates are used.
- $\operatorname{Det}(A^T) = \operatorname{Det}(A)$.
  $\operatorname{Det}(A^{-1}) = 1/\operatorname{Det}(A)$.
  $\operatorname{Det}(A \cdot B) = \operatorname{Det}(A) \cdot \operatorname{Det}(B)$.

The MATLAB function for computing the determinant of matrix M is, not surprisingly, `det(m)`.

```
>> det([1,2,3; 4,0,-1; -3,-2,-4])
ans =
    12
```

6.4.8 Coordinate transformation on image arrays

If A is an image array, so that $A[i, j]$ is the grey scale at the pixel at location i, j, then it is often desirable to apply the geometric transformation discussed to the image. The same formulas apply, of course, but they have to be apply to the *indices* i, j rather than to the values. (Changes to the values give image operations like brightening, changing color, or heightening contrast.)

Suppose you have an $m \times n$ image array A of square pixels. Let us consider the coordinate system whose origin is at the top left-hand corner, whose unit length is the size of a pixel, x coordinate is horizontal, and y coordinate is vertically down (top to bottom, because that is the way MATLAB prints matrices). The image consists of a non-white figure against a white ground. You wish to apply to the figure a linear transformation, whose matrix in homogeneous coordinates is M, filling in any gaps with white, and cropping any part of the figure that lies outside the canvas. To a very crude first approximation, the following MATLAB code will work:

```
function B = TransformImage(M,A);
  white = 255; % gray level for white.
  [n,m] = size(A);
  for i = 1:n
    for j = 1:m
      B(i,j) = white;
     end
  end
  for i = 1:n
    for j = 1:m
      v = floor(M*[i;j;1])
      if (1 <= v(1) & v(1) <= n & 1 <= v(2) & v(2) <= m & A(i,j) ~= white)
        B(v(1),v(2)) = A(i,j);
      end
    end
  end
end
```

The problem with this, however, is that except in very specific cases, a pixel in B does not correspond to a single pixel in A; it overlaps with the image of several pixels in A. The only cases where there

is a one-to-one correspondence are when M is a translation by a pair of integers; M is a rotation by a multiple of 90°; M is a reflection around the coordinate axes; or M is a composition of these. In any other case, the result of the simple algorithm above will probably look seriously wrong. The fixes to this are beyond the scope of this book; see, for example (Foley and van Dam, 1990, section 17.4).

Exercises

Use MATLAB as needed.

Exercise 6.1

Represent the plane containing the points $\langle 2, 0, 1\rangle$, $\langle -1, 1, 1\rangle$ $\langle 1, 1, 0\rangle$ in the form $\{\vec{p} \,|\, \vec{p} \cdot \vec{w} = c\}$.

Exercise 6.2

Find the projection from the point $\langle 3, 3, 3\rangle$ on the plane in exercise 1 and find the distance from the point to the plane.

Exercise 6.3

Find an orthonormal basis for the plane in exercise 1.

Exercise 6.4

Find the intersection of the plane in exercise 1 with the line $\langle 1, 1, 0\rangle + t \cdot \langle 2, 1, 1\rangle$

Exercise 6.5

The intersection of the plane in exercise 1 with the plane $x + y + 2z = 4$ is a line. Characterize this line in the form $\mathbf{p} + t\vec{\vec{w}}$.

Exercise 6.6

For each matrix M listed below, consider the product $M \cdot \vec{v}$ where $\vec{v}$ is the homogeneous coordinates of a point in two-space. State whether this operation carries out a translation, rigid motion, scale transformation, invertable affine transformation, or degenerate affine transformation; whether or not it leaves the origin fixed; and whether or not it is a reflection. Note that $|\langle 0.28, 0.96\rangle| = 1$. Given that fact, you should be able to do these by inspection, without putting pencil to paper, let alone running MATLAB.

Draw a sketch of what the operations looks like.

$$\begin{bmatrix} 0.28 & -0.96 & 0 \\ 0.96 & 0.28 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \begin{bmatrix} 0.28 & 0.96 & 1 \\ -0.96 & 0.28 & 3 \\ 0 & 0 & 1 \end{bmatrix} \qquad \begin{bmatrix} 0.96 & 0.28 & 3 \\ 0.28 & -0.96 & 2 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 3 \\ 0 & 1 & 2 \\ 0 & 0 & 1 \end{bmatrix} \qquad \begin{bmatrix} 2.8 & -9.6 & 0 \\ 9.6 & 2.8 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \begin{bmatrix} 0.96 & 0.28 & 0 \\ 0.28 & 0.96 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 0 & 0 & 1 \end{bmatrix} \qquad \begin{bmatrix} 1 & 2 & 0 \\ 4 & 8 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Problems

Problem 6.1

Give geometric proofs of the equations on p. 124.

Problem 6.2

Let $\vec{u}$ and $\vec{v}$ be two three-dimensional vectors, and let $\vec{w} = \vec{u} \times \vec{v}$ be their cross-product, as defined on p. 129.

A. Prove that $\vec{w} = \vec{0}$ if and only if $\vec{u}$ and $\vec{v}$ are parallel.

B. Prove that $\vec{w}$ is orthogonal to both $\vec{u}$ and $\vec{v}$.

Problem 6.3

In figure 6.15, assuming that the coordinate system on the left has unit length, what is the area of the parallelogram on the right? What is the area of the ellipse? Recall that, as stated in section 6.4.5, the transformation matrix is

$$M = \begin{bmatrix} 1/4 & -1/2 \\ 1/2 & 1 \end{bmatrix}$$

Programming Assignments

Assignment 6.1: Pappus' theorem

A. Write a function `QuadIntersect(A,B,C,D)` that takes as arguments four points `A,B,C,D` and returns the coordinates of the intersection of the line containing `A` and `B` with the line containing `C` and `D`. Don't worry about checking for special cases e.g. there is no line because `A == B` or the two lines are parallel.[6]

For example `QuadIntersect([0,0],[1,1],[1,0],[0,1])` should return `[0.5,0.5]`. `QuadIntersect([0,0], [10,0], [0,5], [-1,4])` should return `[0,-5]`.

[6]The writer of this textbook is here encouraging utterly irresponsible behavior. Not checking for special cases is very bad programming style; one of the hallmarks of production quality software as opposed to immature software is "failing gracefully"; that is, returning meaningful values and generating useful error/warning messages for erroneous or otherwise improper inputs. However, in geometric programming especially, there tend to be lots of special cases, and it can be very difficult to find them all and to decide what should be done. The code for handling special cases can easily be several times longer than the code for handling the standard case. The object of the assignments in this course is to teach the mathematics and to give students practice in rapid prototyping, not to teach high-quality software engineering.

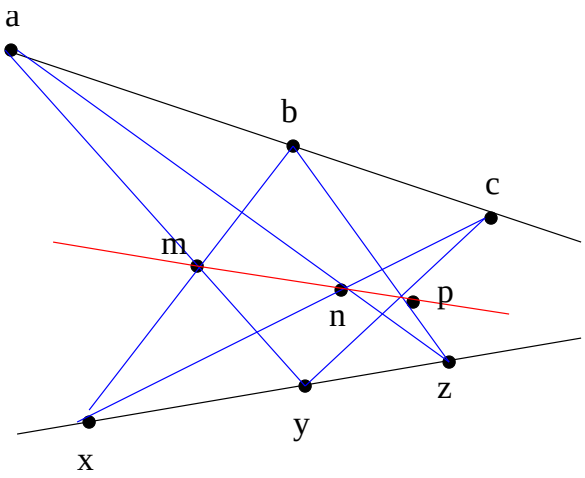


Figure 6.17: Pappus' theorem

B. Pappus' theorem states the following: Suppose that points **a,b,c** lie on one line and points **x,y,z** lie on another. Construct the following points:

> **m** is the intersection of lines **ay** and **bx**. **n** is the intersection of lines **az** and **cx**. **p** is the intersection of lines **bz** and **cy**.

Then **m,n,p** lie on a line (Figure 6.17).

Write a function `RandomPappus` with no arguments that generates a random diagram illustrating Pappus' theorem. That is, construct random points **a,b,x,y**; construct a random point **c** on **ab** and a random point **z** on **xy**, and then construct the corresponding diagram. Note: in rare cases the calculation may fail; more commonly, the diagram may end up so ugly as to be useless. Do not worry about these.

Curious observation: If you use the MATLAB rank function to check whether **m,n,p** are collinear, using the default tolerance — that is, you set up the matrix with row $\mathbf{p}-\mathbf{m}$ and $\mathbf{n}-\mathbf{m}$ and check whether it has rank 1 — it fails 16% of the time. We will discuss the issues involved here in section 7.9.2.

Assignment 6.2

Write a function `CircumscribeTriangle(A,B,C)` that takes as input the coordinates of three points in the plane, `A,B,C`, draws the triangle connecting them and the circumscribing circle (the circle that goes through all three points).

The center of the circumscribing circle is the intersection of the perpendicular bisectors to the sides. Therefore, it can be computed as follows:

- Find the midpoint **x** of side **ab**.
- Find the midpoint **y** of side **bc**.
- Find the line L through **x** perpendicular to **ab**.
- Find the line M through **y** perpendicular to **bc**.

- Find the intersection **o** of L with M. (If **a,b** and **c** are collinear, then there is no intersection and MATLAB will give an error at this point.)
- Let r be the distance from **o** to **a**. Then the circle centered at **o** of radius r is the circumscribing circle.

To draw a circle of center **o** and radius r, compute the points $\mathbf{o} + r \cdot \langle \sin(2\pi t/N), \cos(2\pi t/N) \rangle$ for $t = 1 \ldots N$ for some large N (e.g. $N = 100$).

Figure 6.18 shows the drawing for the function call `CircumscribeTriangle([0,0], [3,0], [1,2])`

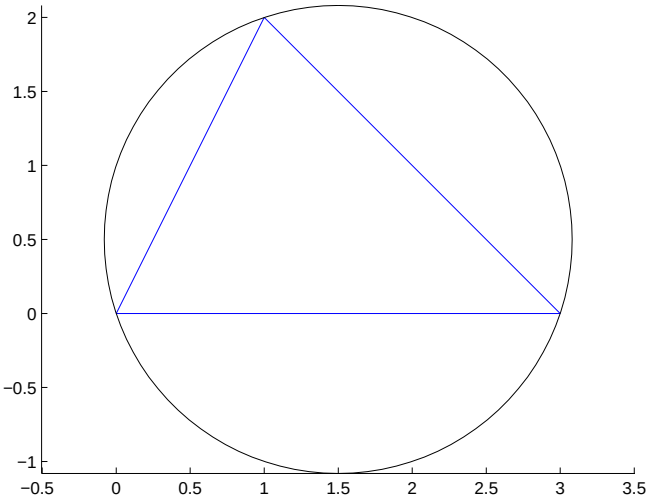


Figure 6.18: `CircumscribeTriangle([0,0], [3,0], [1,2])`

Assignment 6.3: Rotating a Polyhedron

In this assignment, you will use MATLAB to show how the appearance of a 3D object changes as a result of rotation (assuming that the distance to the object is constant, and large as compared to the size of the object).

We will greatly simplify the problem by restricting it to *convex polyhedra.* The advantage of using a convex polyhedron is that it is easy to determine what parts of the surface are visible; a face of a convex polyhedron is visible if the normal to the face points toward the viewer.

The assigment is to write a function `DrawRotatedPolyhedron(M,P)`. The input parameters are M, a 3x3 rotation (orthogonal) matrix, and P, a data structure representing a convex polyhedron. What the function does is to draw a two-dimensional picture of P after rotation by M in a form to be described below.

The input data structure representing of an n-face polyhedron P is a cellular array of size n, where each cell is a face of the polyhedron. A face of the polyhedron with k vertices is a $3 \times k$ array where each column of the array contains the coordinates of the vertices. The columns are in counter-clockwise order, as viewed by someone outside the solid looking at the face.

For example, the unit cube is represented as a cellular array { X1,X2,Y1,Y2,Z1 Z2 } where X1 is the

face at the low end of the x-axis, X2 is the face at the high end of the x-axis, and so on. Specifically,

$$X1 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \qquad X2 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix} \qquad Y1 = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}$$

$$Y2 = \begin{bmatrix} 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \qquad Z1 = \begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \qquad Z2 = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

This and other shapes are defined as scripts in file *polyhedra.m*. The function `EulerRotation(Psi,Phi,Theta)` generates the 3D rotation with Euler angles Psi, Phi, Theta.

The picture of the shape will reflect the appearance of the rotated shape as seen from below; thus, the projection of the faces that are visible below onto the x-y plane (see figure). The picture will show (1) the visible vertices and edges (2) in the center of each face, the projection of a small circle around the center (which will project as an ellipse).

Constructing this picture involves the following steps:

- Apply the matrix M to each of the points in P, generating a new polyhedron P'. (Since the absolute position of of the polyhedron does not matter, you can use natural coordinates and a 3×3 rotation matrix rather than homogeneous coordinates and a 4×4 matrix.)
- Exclude faces that are not visible from below. To do this, compute the outward normal to each face, and exclude any face whose normal has a positive z-component. To find the outward normal to a face, choose any three consecutive vertices of the face $\mathbf{a}, \mathbf{b}, \mathbf{c}$; the cross-product $(\mathbf{c} - \mathbf{b}) \times (\mathbf{a} - \mathbf{b})$ is the outward normal.
- Project the vertices and edges onto the $x - y$ plane simply by ignoring the z coordinate. Draw these in the picture.
- Compute the central circles on each visible face as follows:
  - Compute the center $\mathbf{o}$ of the face as the average of the vertices of the face.
  - Choose a radius r as half the distance from $\mathbf{o}$ to the nearest of the edges (use the formula for the distance from a point to an edge discussed in class)
  - Find two orthonormal arrows $\vec{\vec{u}}, \vec{\vec{v}}$ in the plane of the face. If $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are vertices in the face, then you can choose $\vec{\vec{u}} = \mathrm{Dir}(\mathbf{b} - \mathbf{a})$ as one and $\vec{\vec{v}} = \mathrm{Dir}(\mathbf{c} - \mathbf{p})$ as the other, where $\mathbf{p}$ is the projection of $\mathbf{c}$ on line $\mathbf{ab}$.
  - Compute points on the circle in 3D as $\mathbf{o} + r\cos(2\pi t/N)\vec{u} + r\sin(2\pi t/N)\vec{v}$ for $t = 0 \ldots N$.
  - Project these points onto the $x - y$ plane by ignoring the z-coordinate, and connect the points to plot the ellipse.

Some sample outputs are shown in figures 6.19–6.22.

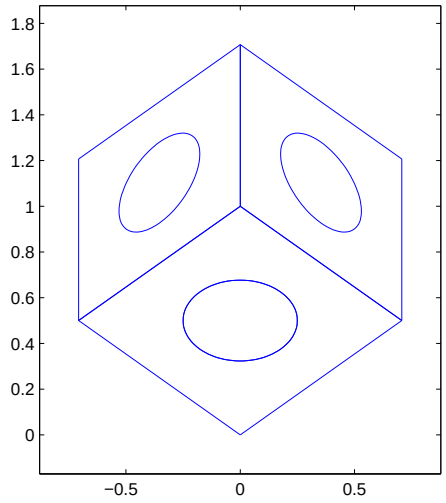


Figure 6.19: `DrawRotatedPolyhedron(EulerRotation(pi/4, pi/4, 0), cube)`

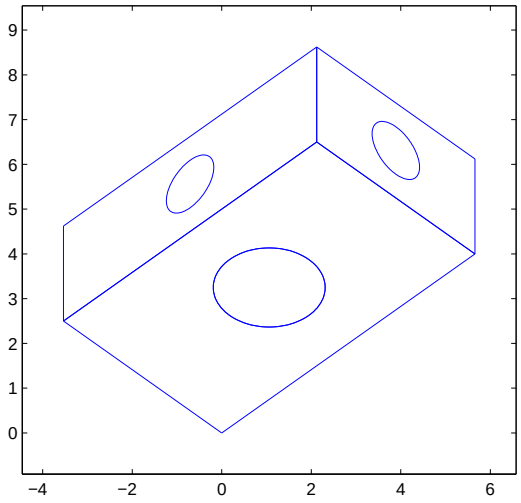


Figure 6.20: `DrawRotatedPolyhedron(EulerRotation(pi/4, pi/4, 0), box)`

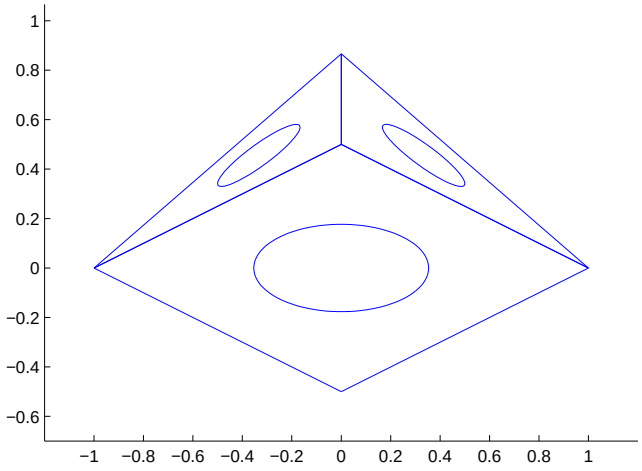


Figure 6.21: `DrawRotatedPolyhedron(EulerRotation(0, pi/3, 0), pyramid)`

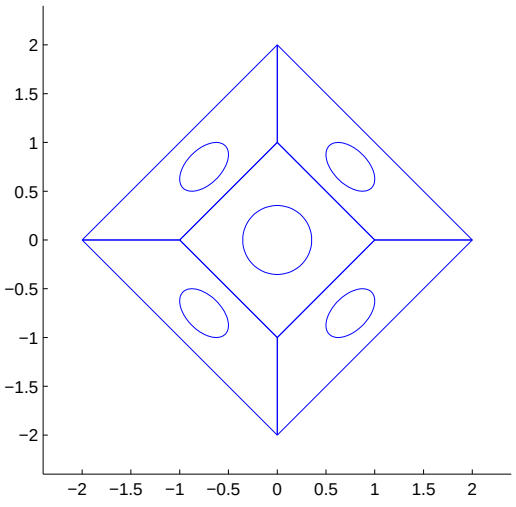


Figure 6.22: `DrawRotatedPolyhedron(EulerRotation(0, pi, 0), frustum)`

Chapter 7

Change of Basis, DFT, and SVD

7.1 Change of coordinate system

Let us return to the first example in chapter 6: We want to record the position of lampposts in a city. So we chose a coordinate system $\mathcal{C}$ with origin $\mathbf{o}$ and coordinate arrows $\vec{x}, \vec{y}$; did lots of measurements; and recorded the positions of all the thousands of lampposts in our city gazeteer.

The day after we finish this, the boss calls us into his office, and tells us he wants to use a different coordinate system $\mathcal{D}$; this one will have origin $\mathbf{q}$, unit length m, and coordinate arrows $\vec{i}$ and $\vec{j}$. Is there a simple way to convert the $\mathcal{C}$ coordinates to $\mathcal{D}$ coordinates?

The solution is simple. All we have to do is to measure the coordinates of $\mathbf{o}$, $\vec{x}$ and $\vec{y}$ in $\mathcal{D}$. Suppose that the coordinates of $\mathbf{o}$ are $\langle a, b\rangle$; the coordinates of $\vec{x}$ are $\langle c, d\rangle$ and and the coordinates of $\vec{y}$ are $\langle e, f\rangle$. Let $\mathbf{p}$ be a point whose coordinates in the $\mathbf{o}, \vec{x}, \vec{y}$ system have been measured to be $\langle s, t\rangle$. Then

$$\mathbf{p} = \mathbf{o} + s\vec{x} + t\vec{y} = (\mathbf{q} + a\vec{i} + b\vec{j}) + s(c\vec{i} + d\vec{j}) + t(e\vec{i} + f\vec{j}) =$$
$$\mathbf{q} + (a + sc + te)\vec{i} + (b + sd + td)\vec{j}$$

Using homogeneous coordinates, we can write this,

$$\mathrm{Hc}(\mathbf{p}, \mathcal{D}) = \begin{bmatrix} c & e & a \\ d & f & b \\ 0 & 0 & 1 \end{bmatrix} \cdot \mathrm{Hc}(\mathbf{p}, \mathcal{C})$$

That is, the conversion from homogeneous coordinates in $\mathcal{C}$ to $\mathcal{D}$ coordinates is just a linear transformation.

For example, suppose $\mathrm{Coords}(\mathbf{o}, \mathcal{D}) = \langle 1, 2\rangle$, $\mathrm{Coords}(\vec{x}, \mathcal{D}) = \langle 3, 2\rangle$, $\mathrm{Coords}(\vec{y}, \mathcal{D}) = \langle -2, 3\rangle$, and suppose $\mathrm{Coords}(\mathbf{p}, \mathcal{C}) = \langle 2, 1\rangle$ (figure 7.1). Then

$$\mathrm{Hc}(\mathbf{p}, \mathcal{D}) = \begin{bmatrix} 3 & -2 & 1 \\ 2 & 3 & 2 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 5 \\ 9 \\ 1 \end{bmatrix}$$

Conversely, to convert from coordinates in $\mathcal{D}$ to coordinates in $\mathcal{C}$, we can solve the corresponding

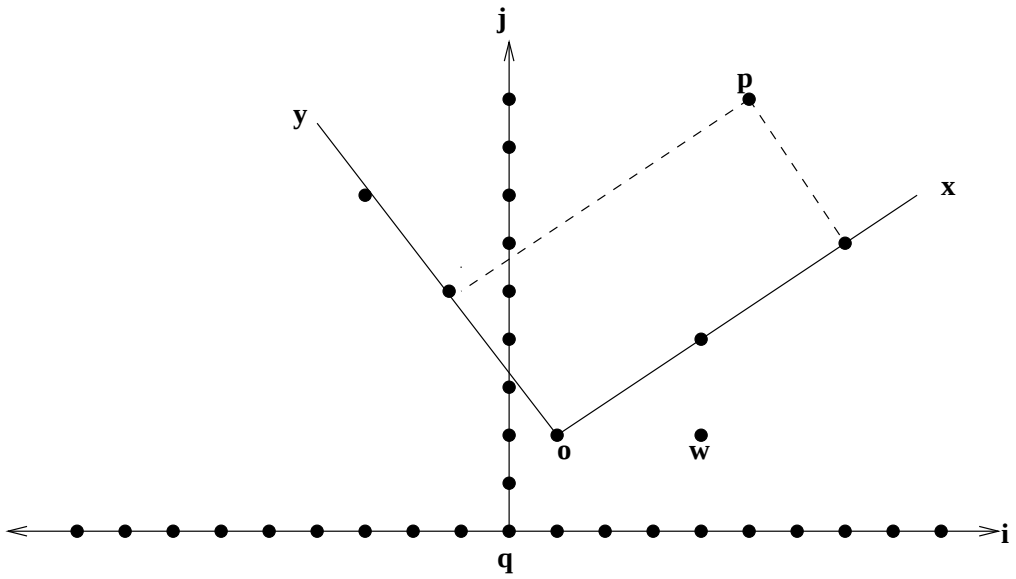


Figure 7.1: Coordinate Transformation

system of linear equations. For instance, with the above coordinate systems, if $\text{Coords}(\mathbf{w}, \mathcal{D}) = \langle 4, 2\rangle$ then we have

$$\begin{bmatrix} 3 & -2 & 1 \\ 2 & 3 & 2 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} \mathbf{w}[x] \\ \mathbf{w}[y] \\ 1 \end{bmatrix} = \begin{bmatrix} 4 \\ 2 \\ 1 \end{bmatrix}$$

So $\text{Coords}(\mathbf{w}, \mathcal{C}) = \langle 9/13, -6/13\rangle$.

If the two coordinate system have the same origin, then natural coordinates can be used instead of homogeneous coordinates. The analysis is the same.

7.1.1 Affine coordinate systems

We skipped a step just now. In chapter 6 we required that the coordinate arrows $\vec{x}$ and $\vec{y}$ have the same (unit) length, and be perpendicular. But in the calculation we just did, we didn't require that that hold for either $\vec{x}, \vec{y}$ or for $\vec{i}, \vec{j}$. What is the meaning of a coordinate system in which the coordinate vectors are not the same length and are not perpendicular?

Such a coordinate system is known as an *affine* coordinate system, and can be defined as long as the two coordinate vectors are not parallel. Let $\mathcal{C}$ be an affine coordinate system with origin $\mathbf{o}$, and coordinate vectors $\vec{x}, \vec{y}$. Then the coordinates of a point $\mathbf{p}$ is the pair $\langle a, b\rangle$ such that $\mathbf{p} = \mathbf{o} + a\vec{x} + b\vec{y}$. These can be found using the following procedure. Let L and M be the two coordinate axes $L = \{\mathbf{o} + t\vec{x} | t \in \mathbb{R}\}$ and $M = \{\mathbf{o} + t\vec{y} | t \in \mathbb{R}\}$. Draw the line parallel to M through $\mathbf{p}$ and let $\mathbf{q}$ be the point where this intersects L; and draw the line parallel to L through $\mathbf{p}$ and let $\mathbf{r}$ be the point where this intersects L. Then $a = (\mathbf{q} - \mathbf{p})/\vec{x}$ and $b = (\mathbf{r} - \mathbf{p})/\vec{y}$. For instance, in figure 7.2 $a = 3$ and $b = 2$. Note that if $\vec{x}$ and $\vec{y}$ are orthogonal then the line parallel to M is the perpendicular to L, which is how we defined this construction in section 6.2, but in the general case, we use the parallels rather than the perpendiculars.

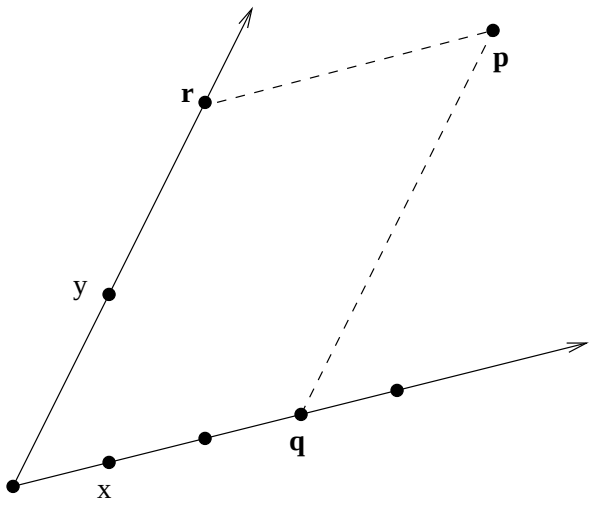


Figure 7.2: Affine Coordinates

The analogous construction applies to affine coordinate systems in three-space except that the condition that $\vec{x}$ and $\vec{y}$ are not parallel is replaced by the condition that $\vec{x}$, $\vec{y}$, and $\vec{z}$ are not coplanar.

Addition of vectors in affine coordinate systems works as usual:

$$\text{Coords}(\mathbf{p} + \vec{v}, \mathcal{C}) = \text{Coords}(\mathbf{p}, \mathcal{C}) + \text{Coords}(\vec{v}, \mathcal{C}).$$
$$\text{Coords}(\vec{u} + \vec{v}, \mathcal{C}) = \text{Coords}(\vec{u}, \mathcal{C}) + \text{Coords}(\vec{v}, \mathcal{C}).$$
$$\text{Coords}(c \cdot \vec{v}, \mathcal{C}) = c \cdot \text{Coords}(\vec{v}, \mathcal{C}).$$

However, the dot product formulas no longer work properly for computing lengths, distances, and angles.

7.1.2 Duality of transformation and coordinate change; Handedness

The changes of coordinate system discussed above and the geometric transformations discussed in section 6.4 create the same kind of changes to coordinates in ways that are dual to one another, in the following sense. Suppose that on Sunday Ed records that the corners of the dining room table are located at coordinates $\langle 2, 3\rangle, \langle 5, 3\rangle, \langle 5, 4\rangle, \langle 2, 4\rangle$. On Monday, Dora records that the corners are at $\langle 8, 6\rangle, \langle 11, 6\rangle, \langle 11, 7\rangle, \langle 8, 7\rangle$. Then one possibility is that the table has undergone a translation by $\langle 6, 3\rangle$. Another possibility is that Dora is using a different coordinate system, one with the same coordinate directions and unit length, but with an origin whose coordinates in Ed's system are $\langle -6, -3\rangle$. (Or, of course, there may have been both a transformation and a change of coordinate system; but we are interested in comparing the two pure cases.)

So there is a correspondence between transformations and changes of coordinate systems and between categories of transformations and categories of coordinate system changes. In particular:

- As in the above example, a translation by $\langle x, y\rangle$ corresponds to moving the origin by $\langle -x, -y\rangle$. The directions and unit length of the coordinate system remain unchanged.
- A pure rotation corresponds to rotating the coordinate system in the opposite direction. In particular, an orthonormal coordinate system is changed to another orthonormal coordinate system.

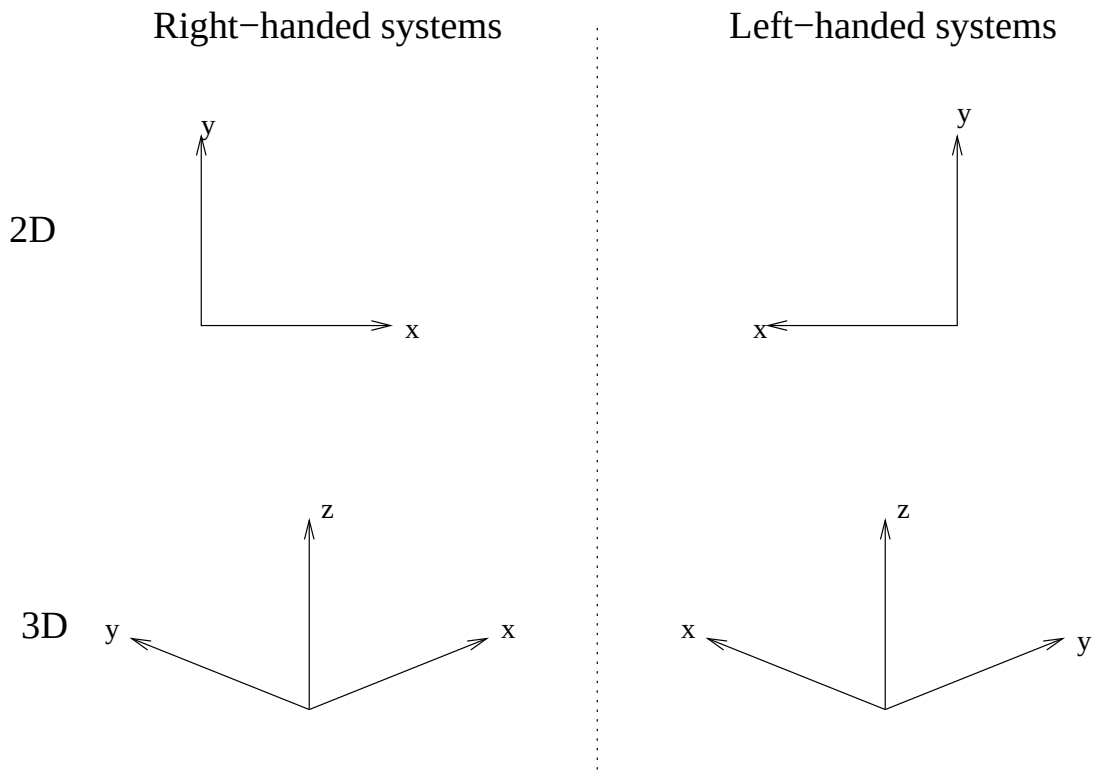


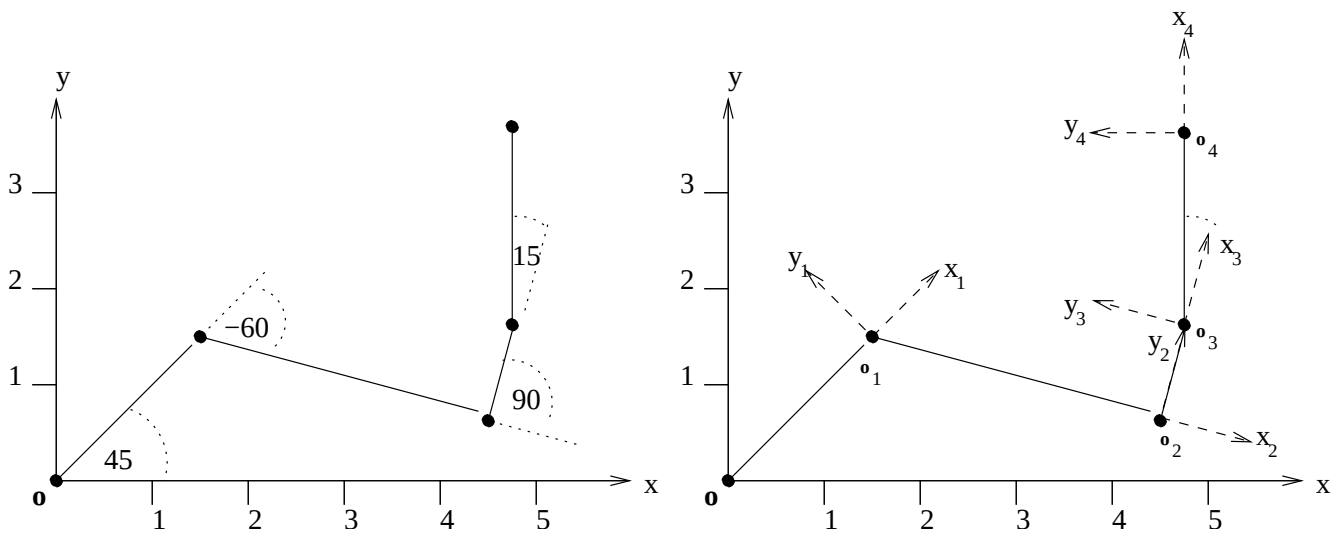
Figure 7.3: Right- and left-handed coordinate systems

- A expansion by c corresponds to a contraction of the unit length of the coordinate system by c. The origin and coordinate directions remain unchanged.

Reflections are more interesting. A reflection corresponds to changing to changing the handedness of the coordinate system; changing a left-handed coordinate system into a right-handed one, or vice versa (figure 7.3). In the plane, a right-handed coordinate system places the y-axis 90° counterclockwise from the x-axis; a left-handed coordinate system places the y axis clockwise from the x-axis. In a right-handed coordinate system in three-space, the axes are aligned so that, if you place your right hand along the x axis, pointing your fingers in the positive x direction, and your palm is facing in the positive y direction, then your thumb is pointing in the positive z-direction. In a left-handed coordinate system, the same holds with your left hand.

Unlike other properties of bases that we have considered, the handedness of a coordinate system depends on the *order* of the basis elements and not just on the set of coordinate vectors. If $\langle \hat{x}, \hat{y} \rangle$ is a right-handed coordinate system, then $\langle \hat{y}, \hat{x} \rangle$ is a left-handed coordinate system; it corresponds (in the above sense) to the reflection across the line $x = y$. In three dimensions, if $\langle \hat{x}, \hat{y}, \hat{z} \rangle$ is a right-handed coordinate system then $\langle \hat{y}, \hat{z}, \hat{x} \rangle$ and $\langle \hat{z}, \hat{x}, \hat{y} \rangle$ are also right-handed; whereas $\langle \hat{y}, \hat{x}, \hat{z} \rangle$, $\langle \hat{x}, \hat{z}, \hat{y} \rangle$, and $\langle \hat{z}, \hat{y}, \hat{x} \rangle$ are left-handed.

The distinction between right- and left-handed coordinate systems — or, more precisely, between a pair of coordinate systems with the same handedness and a pair with opposite handedness — carries over into higher dimensions. In any dimension, any coordinate system has one of two handednesses. Swapping the order of two vectors in the basis flips the handedness; doing a second swap restores it. For instance, let $\mathcal{B} = \langle \vec{b}_1, \vec{b}_2, \vec{b}_3, \vec{b}_4, \vec{b}_5 \rangle$ be a basis in $\mathbb{R}^5$. Let $\mathcal{C} = \langle \vec{b}_1, \vec{b}_4, \vec{b}_3, \vec{b}_2, \vec{b}_5 \rangle$ be the result of swapping the second and fourth vector in $\mathcal{B}$. Then $\mathcal{C}$ has the opposite handedness to $\mathcal{B}$. Let $\mathcal{D}$



$L_1 = 2.\ L_2 = 3.\ L_3 = 1.\ L_4 = 2.$
$\theta_1 = 45°.\ \theta_2 = -60°.\ \theta_3 = 90°.\ \theta_4 = 15°.$

Figure 7.4: Two dimensional robotic arm

be the result of swapping the second and fifth vector in $\mathcal{C}$: $\mathcal{D} = \langle \vec{b}_1, \vec{b}_5, \vec{b}_3, \vec{b}_2, \vec{b}_4 \rangle$. Then $\mathcal{D}$ has the opposite handedness to $\mathcal{C}$, and the same handedness as $\mathcal{B}$.

7.1.3 Application: Robotic arm

Simple robotic arms can be analyzed using coordinate transformations. We will model a robotic arm as a sequence of k links, each of a fixed length, with a pin joint between successive links that allows rotation in the plane perpendicular to the pin. The first link is attached to the origin by a pin joint. The robot directly controls the angles $\theta_1 \ldots \theta_k$, where θ_1 is the angle in the $x-y$ plane of the first link, and for $i > 1$, θ_i is the angle between the forward directions on the $i-1$st link and the ith link (figure 7.4). The question is, for a given sequence of angles $\theta_1 \ldots \theta_k$, what is the position of the end of the last link, and what is the direction of the last link?. (The inverse problem — given a target position and direction, find a sequence of angles that achieves it — is known as the "inverse kinematics" problem, and is a hard problem, beyond the scope of this book.)

Let us consider first the 2D case, in which all the pins are vertical, and hence all the links rotate in the $x-y$ plane, like a folding yardstick. In this case, we can ignore the vertical dimension altogether. We will solve the problem by attaching a little coordinate system $\mathcal{C}_i$ with origin $\mathbf{o}_i$ and coordinate directions $\vec{\vec{x}}_i$ and $\vec{\vec{y}}_i$ to the end of ith link where $\vec{\vec{x}}_i$ points in the direction of the link. $\mathcal{C}_0$ is the external, absolute, coordinate system. Let L_i be the length of the ith link. Then for $i = 1 \ldots k$ we have the following relations:

- $\vec{\vec{x}}_i$, $\vec{\vec{y}}_i$ are rotated by θ_i from $\vec{\vec{x}}_{i-1}$, $\vec{\vec{y}}_{i-1}$.
- $\mathbf{o}_i$ is located at $\mathbf{o}_{i-1} + L_i \cdot \vec{\vec{x}}_i$.

It would seem at first[1] that one could view this problem in terms of a sequence of geometric trans-

[1]To be precise, I originally wrote this section using geometric transformations, and was surprised to find that I

formations from $\mathcal{C}_0$ to $\mathcal{C}_1$ to $\mathcal{C}_2$ .... But that doesn't work, because geometric transformations are measured with respect to the absolute coordinate system $\mathcal{C}_0$, whereas here we are given the coordinate of $\mathcal{C}_2$ in terms of $\mathcal{C}_1$, and of $\mathcal{C}_3$ in terms of $\mathcal{C}_2$. So we have to combine coordinate transformations. What we will do is find the coordinate transformation from $\mathcal{C}_n$ to $\mathcal{C}_{n-1}$, from $\mathcal{C}_{n-1}$ to $\mathcal{C}_{n-2}$, ... from $\mathcal{C}_1$ to $\mathcal{C}_0$; and compose them to get the coordinate transformation from $\mathcal{C}_n$ to $\mathcal{C}_0$. Since the coordinate transformation is the inverse of the geometric transformation, this composition will give the coordinates of $\mathcal{C}_n$ in $\mathcal{C}_0$.

We will represent the coordinate transformation from $\mathcal{C}_n$ to $\mathcal{C}_i$ in homogeneous coordinates in terms of a matrix

$$T_i = \left[\begin{array}{c|c} R_i & \vec{v}_i \\ \hline \vec{0}^T & 1 \end{array}\right]$$

The coordinate transformation from $\mathcal{C}_i$ to $\mathcal{C}_{i-1}$ consists of two parts in sequence.

1. A translation of the origin by $-L_i\vec{\vec{x}}$, relative to the coordinate system $\mathcal{C}_i$. Let us call this intermediate coordinate system $\mathcal{D}_i$. The corresponding coordinate transformation matrix is

$$\begin{bmatrix} 1 & 0 & L_i \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

2. A rotation by $-\theta_i$ around the origin of $\mathcal{D}_i$. The corresponding coordinate transformation is

$$\begin{bmatrix} \cos(\theta_i) & -\sin(\theta_i) & 0 \\ \sin(\theta_i) & \cos(\theta_i) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Therefore, the combined transformation from $\mathcal{C}_i$ to $\mathcal{C}_{i-1}$ is the composition of these two:

$$T_i = \begin{bmatrix} \cos(\theta_i) & -\sin(\theta_i) & 0 \\ \sin(\theta_i) & \cos(\theta_i) & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & L_i \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} \cos(\theta_i) & -\sin(\theta_i) & L_i\cos(\theta_i) \\ \sin(\theta_i) & \cos(\theta_i) & L_i\sin(\theta_i) \\ 0 & 0 & 1 \end{bmatrix}$$

The coordinate transformation from $\mathcal{C}_n$ to $\mathcal{C}_0$ is then the composition of all of these $T_1 \cdot T_2 \cdot \ldots T_n$. The upper left 2×2 square gives the rotation of $\mathcal{C}_n$ from $\mathcal{C}_0$ and the first two elements in the third column give the coordinates of $\mathbf{o}_n$ in terms of $\mathcal{C}_0$.

Now actually in the two dimensional case, we could have done this more simply without the matrix algebra, because in two dimensions, rotational angles simply add. Define $\phi_1 = \theta_1$, $\phi_2 = \theta_1 + \theta_2$, $\phi_3 = \theta_1 + \theta_2 + \theta_3$, and so on up to $\phi_n = \theta_1 + \ldots + \theta_n$. Then ϕ_i is the total rotation between $\mathcal{C}_0$ and $\mathcal{C}_i$. The arrow, in absolute coordinates, from $\mathbf{o}_{i-1}$ to $\mathbf{o}_i$ is $\langle L_i\cos(\phi_i), L_i\sin(\phi_i)\rangle$ so the coordinates of $\mathbf{o}_n$ in $\mathcal{C}_0$ is

$$\langle L_1\cos(\phi_1) + L_2\cos(\phi_2) + \ldots + L_n\cos(\phi_n), L_1\sin(\phi_1) + L_2\sin(\phi_2) + \ldots + L_n\sin(\phi_n)\rangle$$

Moving on to the three-dimensional case, however, there is no alternative to using matrix algebra. Let us consider the following model of an arm.[2]. Again, the arm consists of n links of length $L_1 \ldots L_n$ connected in sequence by pin joints. The angle at the connection between the $i-1$st and ith links is

was getting the wrong answers. It took me 15 minutes of thought to work out what the problem was; a fine example of how the kind of confusion discussed in section 7.3 can arise even in very concrete, geometric applications.

[2]I do not know of any actual arm built like this, but it is a convenient model

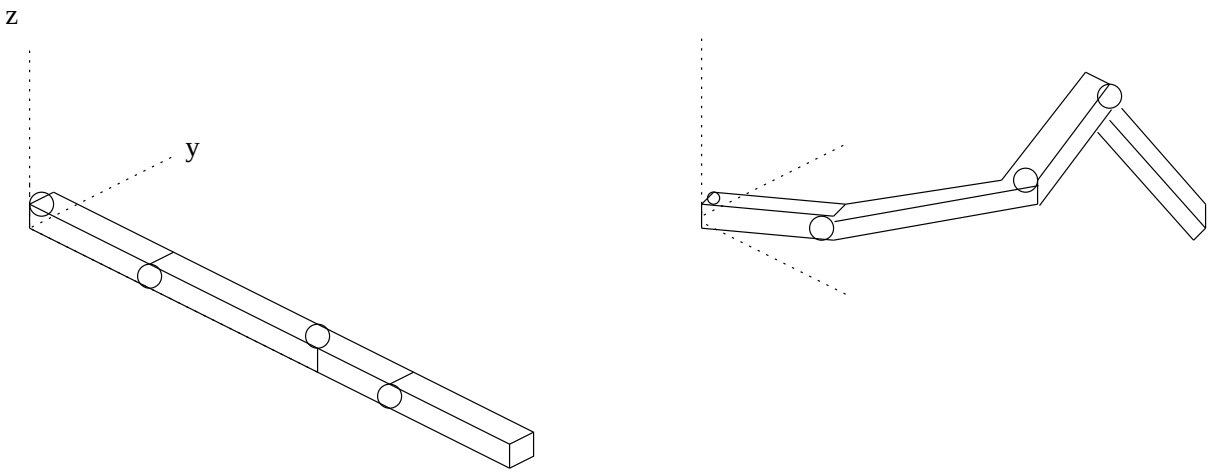


Figure 7.5: Three dimensional robotic arm

θ_i and when all the θ_i are zero, then the links lie stretched out along the positive x-axis. However, the direction of the pins alternates. Specifically, the pin at the origin is always vertical, so that the first link rotates in the $x-y$ plane. When $\theta_1 = 0$ the second pin is parallel to the y axis, so the second link rotates in the $x-z$ plane. When all the θ's are 0 the third pin is again vertical, the fourth pin is again parallel to the y axis, the fifth is vertical, the sixth is parallel to the y axis and so on. (Figure 7.5)

The linear algebra is essentially the same as in the two dimensional case. Again we attach a little coordinate system $\mathcal{C}_i$ to the far end of the ith link, and we will compute the coordinate transformation from $\mathcal{C}_n$ to $\mathcal{C}_0$ using matrix multiplication using homogeneous coordinates. The only difference is in the rotations.

As in the two-dimensional case, the transformation from $\mathcal{C}_i$ to $\mathcal{C}_{i-1}$ consists of two parts:

- Translating the origin by $-L_i\vec{\vec{x}}$. The corresponding matrix is

$$\begin{bmatrix} 1 & 0 & 0 & L_i \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- If i is even, rotating about the $\vec{\vec{z}}$ axis of $\mathcal{D}_i$. The corresponding matrix is

$$\begin{bmatrix} \cos(\theta_i) & -\sin(\theta_i) & 0 & 0 \\ \sin(\theta_i) & \cos(\theta_i) & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

  If i is odd, rotating about the $\vec{\vec{y}}$ axis of $\mathcal{D}_i$. The corresponding matrix is

$$\begin{bmatrix} \cos(\theta_i) & 0 & -\sin(\theta_i) & 0 \\ 0 & 1 & 0 & 0 \\ \sin(\theta_i) & 0 & \cos(\theta_i) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

If i is even, then the composition of the two transformations is

$$T_i = \begin{bmatrix} \cos(\theta_i) & -\sin(\theta_i) & 0 & 0 \\ \sin(\theta_i) & \cos(\theta_i) & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 0 & L_i \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} \cos(\theta_i) & -\sin(\theta_i) & 0 & L_i\cos(\theta_i) \\ \sin(\theta_i) & \cos(\theta_i) & 0 & L_i\sin(\theta_i) \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

If i is odd, then the composition of the two is

$$T_i = \begin{bmatrix} \cos(\theta_i) & 0 & -\sin(\theta_i) & 0 \\ 0 & 1 & 0 & 0 \\ \sin(\theta_i) & 0 & \cos(\theta_i) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 0 & L_i \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} \cos(\theta_i) & 0 & -\sin(\theta_i) & L_i\cos(\theta_i) \\ 0 & 1 & 0 & 0 \\ \sin(\theta_i) & 0 & \cos(\theta_i) & L_i\sin(\theta_i) \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

The net transformation from $\mathcal{C}_n$ to $\mathcal{C}_0$ is the product $T = T_1 \cdot T_2 \cdot \ldots \cdot T_n$. The upper 3×3 block of T is the net rotation from $\mathcal{C}_0$ to $\mathcal{C}_n$. The first three elements of the right hand column of T are the absolute coordinates of $\mathbf{o}_n$.

7.2 The formula for basis change

We now move from the geometric case to the general case of n-dimensional vectors. Suppose that we have two bases $\mathcal{B}$ and $\mathcal{C}$ for $\mathbb{R}^n$ and we are given the coordinates of vector $\vec{v}$ in $\mathcal{B}$. How can we calculate the coordinates of $\vec{v}$ in $\mathcal{C}$? Theorem 7.2 gives the answer in the case where either $\mathcal{B}$ or $\mathcal{C}$ is the standard basis $\{e^1 \ldots e^n\}$; corollary 7.3 gives the answer in general. First we prove lemma 7.1 which gives a general answer, but not in terms that can immediately be computed.

Lemma 7.1. *Let $\mathcal{V}$ be an n-dimensional vector space. Let $\mathcal{B} = \vec{b}_1 \ldots \vec{b}_n$ and $\mathcal{C} = \vec{c}_1 \ldots \vec{c}_n$ be two ordered bases for $\mathcal{V}$. Define the $n \times n$ matrix M such that $M[;j] = \text{Coords}(\vec{b}_j, \mathcal{C})$. Then, for any vector $\vec{v}$ in $\mathcal{V}$,*

$$\text{Coords}(\vec{v}, \mathcal{C}) = M \cdot \text{Coords}(\vec{v}, \mathcal{B})$$

Proof: Let $\text{Coords}(\vec{v}, \mathcal{B}) = \langle a_1 \ldots a_n \rangle$. Then

$$\vec{v} = a_1\vec{b}_1 + \ldots + a_n\vec{b}_n =$$

$$a_1 \cdot (M[1,1] \cdot \vec{c}_1 + M[2,1] \cdot \vec{c}_2 + \ldots + M[n,1] \cdot \vec{c}_n) +$$
$$a_2 \cdot (M[1,2] \cdot \vec{c}_1 + M[2,2] \cdot \vec{c}_2 + \ldots + M[n,2] \cdot \vec{c}_n)$$
$$+ \ \ldots \ +$$
$$a_n \cdot (M[1,n] \cdot \vec{c}_1 + M[2,n] \cdot \vec{c}_2 + \ldots + M[n,n] \cdot \vec{c}_n)$$
$$=$$
$$(M[1,1] \cdot a_1 + M[1,2] \cdot a_2 + \ldots + M[1,n] \cdot a_n) \cdot \vec{c}_1 +$$
$$(M[2,1] \cdot a_1 + M[2,2] \cdot a_2 + \ldots + M[2,m] \cdot a_m) \cdot \vec{c}_2$$
$$+ \ \ldots \ +$$
$$(M[n,1] \cdot a_1 + M[n,2] \cdot a_2 + \ldots + M[n,n] \cdot a_n) \cdot \vec{c}_n$$

So

$$\begin{array}{l}\text{Coords}(\vec{v},\mathcal{C}) = \\ \langle\ M[1,1]\cdot a_1 + M[1,2]\cdot a_2 + \ldots + M[1,n]\cdot a_n, \\ \quad M[2,1]\cdot a_1 + M[2,2]\cdot a_2 + \ldots + M[2,n]\cdot a_n, \\ \qquad , \ldots , \\ \quad M[n,1]\cdot a_1 + M[n,2]\cdot a_2 + \ldots + M[n,n]\cdot a_n \\ \rangle = \\ M \cdot \text{Coords}(\vec{v},\mathcal{B}).\end{array}$$

Theorem 7.2. *Let $\mathcal{C} = \vec{c}_1 \ldots \vec{c}_n$ be a basis for $\mathbb{R}^n$. Let $\vec{u}$ be a vector and let $\vec{v} = \text{Coords}(\vec{u},\mathcal{C})$. Let M be the $n \times n$ matrix whose columns are the vectors in $\mathcal{C}$; $M[;j] = \vec{c}_j$. Then*

A. $\vec{u} = M\vec{v}$

B. $\vec{v} = M^{-1}\vec{u}$.

Proof: The proof of (A) is immediate from lemma 7.1 with $\mathcal{B}$ being the standard basis for $\mathbb{R}^n$, since $\text{Coords}(\vec{c}_j,\mathcal{B}) = \vec{c}_j$. The proof of (B) is immediate from (A).

Corollary 7.3. *Let $\mathcal{B} = \vec{b}_1 \ldots \vec{b}_n$ and $\mathcal{C} = \vec{c}_1 \ldots \vec{c}_n$ be two bases for $\mathbb{R}^n$. Let $\vec{w}$ be a vector. Let B be the matrix whose columns are $\vec{b}_1 \ldots \vec{b}_n$, and let C be the matrix whose columns are $\vec{c}_1 \ldots \vec{c}_n$. Then* $\text{Coords}(\vec{w},\mathcal{C}) = C^{-1}\vec{w} = C^{-1}\cdot B \cdot \text{Coords}(\vec{w},\mathcal{B})$.

Proof: Immediate from theorem 7.2.

7.3 Confusion and how to avoid it

Despite the simple form of theorem 7.2, it can be quite confusing, for several reasons.

In the first place, the whole idea of vectors can seem to be floating off into the ether. We started with a vector $\vec{v}$ being an n-tuple of numbers; that is nice and concrete. But now the same (??) vector $\vec{v}$ is being represented by a m-tuple of coordinates relative to a basis. Moreover, (a) by choosing the vector space and the basis properly, we can get $\vec{v}$ to have any coordinate vector we want (other than the zero vector); and (b) the basis vectors themselves are just tuples of numbers. So in what sense is this the same vector? And what is the difference between two different vectors, if we can use any vector to represent any other vector? And how do we even pin down what the basis vectors mean, when they also are just tuples of numbers and likewise can turn into anything else?

Abstract mathematics of various kinds can trigger this kind of vertigo, though this particular example is an unusually severe one for math that is considered comparatively elementary and concrete. When you are hit by these kinds of feelings, the best thing to do is to stop working at the abstract level and go back to concrete instances; geometric examples are good, because you can draw pictures. As we did in the previous section, you want to be sure to distinguish between the concrete things on the one hand, and their coordinate vectors on the other.

Really, there is nothing more in this indeterminacy than the fact that a person's height may be 6, when measured in feet, and 72, when measured in inches, but it seems more confusing in this abstract setting.

The second source of confusion is that we have now introduced a second form of linear transformation. Previous to this section, a linear transformation was an operation that turned one thing into a different thing; e.g. a basket vector into a price vector, or a population distribution at one time into a different population distribution at a different time. In theorem 7.2, by contrast, the thing remains the same; what is changing is the way we are representing the thing. The same matrix

multiplication is used for both. Again, this is basically the same as the fact that you multiply a height measurement by 12, either when an object gets 12 times taller, or when you change from feet to inches.

The third source of confusion is that it is easy to get the direction of corollary 7.3 backward. To change a coordinate vector in $\mathcal{B}$ to a coordinate vector in $\mathcal{C}$, you multiply by the matrix of coordinates of $\mathcal{B}$ in $\mathcal{C}$, and not vice versa. Again, if you want to change from a measurement in feet to one in inches, you multiply by 12, which is the measure of 1 foot in inches.

7.4 Non-geometric change of basis

A final source of discomfort about these change of bases, in non-geometric applications, is that it is not obvious what is the point of non-standard bases in the first place. In geometry, the choice of coordinate system is largely arbitrary anyway, so it makes sense to go from one to another. But in the kinds of non-geometric applications we have considered, it is much less clear why you would want to do this.

Consider a specific example of shopping baskets; to make things easy, suppose that there are three products: a gallon of milk, a loaf of bread, and a pound of butter. The natural representation for a basket with x gallons of milk, y loaves of bread, and z pounds of butter is using the vector $\langle x, y, z\rangle$. Now, of course, we *can* use any three linearly independent baskets we want as a basis, say,

$\vec{b}_1$ = 2.5 gallons of milk, -4 loaves of bread, and 3 pounds of butter.
$\vec{b}_2$ = -3 gallons of milk, 2 loaves of bread, and 1 pound of butter.
$\vec{b}_3$ = 0 gallons of milk, -6 loaves of bread, and 7 pounds of butter.

And then we *can* represent a basket with 1 gallon of milk as in terms of the coordinate vector $\langle 1, 1/2, -1/2\rangle$. But why is this anything other than perverse?

In fact, there are many different reasons to consider alternative bases; change of basis is as common in applications of linear algebra as actual change, if not more so. We will consider a number of these in the rest of the chapter.

7.5 Color graphics

There are domains other than the geometric where there can be different equally plausible bases for the vector space. One example is color graphics. Color is essentially a three-dimensional vector space;[3] a single color is the sum of three primary colors, each weighted by an intensity. However, different display systems use different sets of primary colors; for instance, a color printer uses a different set from a color terminal. Each triple of primary colors can be considered as a basis for the space of all colors; conversion of the intensity vector for a particular color from one system of primary colors to another is thus a matter of basis change. (This is an idealization; in practice, things are more complicated.)

[3]The dimension is a function of the human eye, which has three different kinds of cones. Pigeons are believed to have five primary colors. Stomatopods, a kind of shrimp, have twelve.

7.6 Discrete Fourier transform (Optional)

The discrete[4] Fourier transform (DFT) is a basis change that is used throughout signal processing and in many other applications. This will require a little work, but it is well worth taking the time.

A simple signal processor has an input $\mathbf{a}(t)$ and an output $\mathbf{g}(t)$, both of which are functions of time. (In this section, we will use boldface letters for functions of time.) The output depends on the input, so $\mathbf{g} = F(\mathbf{a})$ for some function F. Note that $\mathbf{g}(t)$ may depend on the entire signal $\mathbf{a}$ (or at least all of $\mathbf{a}$ prior to t) and not just on the single value $\mathbf{a}(t)$. Many signal processors have the following elegant properties:

1. F is linear. That is, for any inputs $\mathbf{a}$ and $\mathbf{b}$, $F(\mathbf{a}+\mathbf{b}) = F(\mathbf{a}) + F(\mathbf{b})$. For any constant c, $F(c \cdot \mathbf{a}) = c \cdot F(\mathbf{a})$.
2. F is time-invariant. If input $\mathbf{b}$ is the same as $\mathbf{a}$, delayed by δ, then the output for $\mathbf{b}$ is the same as the output for $\mathbf{a}$, delayed by δ. Symbolically. if $\mathbf{b}(t) = \mathbf{a}(t-\delta)$ then $(F(\mathbf{b}))(t) = (F(\mathbf{a}))(t-\delta)$
3. The output to a sinusoidal input is a sinusoid of the same frequency, possibly amplified and time-delayed. That is, if $\mathbf{a}(t) = \sin(\omega t)$, and $\mathbf{g} = F(\mathbf{a})$ then $\mathbf{g}(t) = A(\omega)\sin(\omega t + \delta(\omega))$. As shown, the quantities $A(\omega)$ and $\delta(\omega)$ may depend on the frequency ω but are independent of time t. The quantities $A(\omega)$ and $\delta(\omega)$ are the *frequency response characteristics* of the signal processor.

Condition (3) above may seem rather constrained. However if the amplifier is characterized by a differential equation, which many physical systems are, and if it is damped, meaning that if the input becomes zero, the output eventually dies down to zero, and if it satisfies conditions (1) and (2), then it necessarily satisfies condition (3).

Using the trigonometric identity $\sin(\alpha+\beta) = \sin(\alpha)\cos(\beta) + \sin(\beta)\cos(\alpha)$, we can rewrite the equation in condition (3) as follows:

$$\mathbf{g}(t) = A(\omega)\sin(\omega t + \delta(\omega)) = A(\omega)\cos(\delta(\omega))\sin(\omega(t)) + A(\omega)\sin(\delta(\omega))\cos(\omega(t))$$

Moveover, since $\cos(\alpha) = \sin(\alpha + \pi/2)$ (the cosine is just a time advanced sine) it follows that the response to the input $\cos(\omega t)$ is just $A(\omega)\cos(\delta(\omega))\cos(\omega(t)) - A(\omega)\sin(\delta(\omega))\sin(\omega(t))$.

Now, suppose that we take an input time signal $a(t)$ and the corresponding output time signal $g(t)$ from time $t = 0$ to $t = T$. We choose an even number $2K$ and we will sample both signals at the $2K$ points, $t = T/2K$, $t = 2T/2K$, $t = 3T/2K$ $\ldots t = 2KT/2K = T$. This gives us two vectors $\vec{a}$ and $\vec{g}$ of dimension $2K$. Thus, for $I = 1 \ldots 2K$, $\vec{a}[I] = \mathbf{a}(IT/2K)$ and $\vec{g}[I] = \mathbf{g}(IT/2K)$. In general for any function $\mathbf{f}(t)$ from 0 to T, we will consider the sample of $2K$ points to be the vector $\vec{f}[I] = \mathbf{f}(I \cdot T/2K)$ for $I = 1 \ldots 2K$.

We are now dealing in the space of $2K$ dimensional vectors. We define the following set of vectors $\mathcal{V} = \{\vec{v}_1 \ldots \vec{v}_{2K}\}$.

$\vec{v}_1 = \vec{1}$.
for $I, J = 1 \ldots K$, $\vec{v}_{2J}[I] = \cos(IJ\pi/K)$.
for $I, J = 1 \ldots K-1$, $\vec{v}_{2J+1}[I] = \sin(IJ\pi/K)$

That is: $\vec{v}_1$ is just the 1 vector. The Jth even-numbered vector is a sample of the cosine function $\cos(J\pi t/T)$ and and the Jth odd-numbered vector is a sample of the sine function $\sin(J\pi t/T)$.

For example, with $K = 2$, $2K = 4$, we have

[4]The continuous Fourier transform is also a basis change, but for an infinite-dimensional space of functions.

$\vec{v}_1 = \langle 1, 1, 1, 1\rangle$
$\vec{v}_2 = \langle \cos(\pi/2), \cos(2\pi/2), \cos(3\pi/2), \cos(4\pi/2)\rangle = \langle 0, -1, 0, 1\rangle$.
$\vec{v}_3 = \langle \sin(\pi/2), \sin(2\pi/2), \sin(3\pi/2), \sin(4\pi/2)\rangle = \langle 1, 0, -1, 0\rangle$.
$\vec{v}_4 = \langle \cos(2\pi/2), \cos(4\pi/2), \cos(6\pi/2), \cos(8\pi/2)\rangle = \langle -1, 1, -1, 1\rangle$.

We would seem to be missing the final sine function, but since that would be
$\langle \sin(2\pi/2), \sin(4\pi/2), \sin(6\pi/2), \sin(8\pi/2)\rangle = \langle 0, 0, 0, 0\rangle$,
it is useless.

With $K = 3$, $2K = 6$, we have

$\vec{v}_1 = \langle 1, 1, 1, 1, 1, 1\rangle$
$\vec{v}_2 = \langle \cos(\pi/3), \cos(2\pi/3), \cos(3\pi/3), \cos(4\pi/3), \cos(5\pi/3), \cos(6\pi/3)\rangle =$
$\langle 0.5, -0.5, -1, -0.5, 0.5, 1\rangle$.
$\vec{v}_3 = \langle \sin(\pi/3), \sin(2\pi/3), \sin(3\pi/3), \sin(4\pi/3), \sin(5\pi/3), \sin(6\pi/3)\rangle =$
$\langle 0.866, 0.866, 0, -0.866, -0.866, 0\rangle$.
$\vec{v}_4 = \langle \cos(2\pi/3), \cos(4\pi/3), \cos(6\pi/3), \cos(8\pi/3), \cos(10\pi/3), \cos(12\pi/3)\rangle =$
$\langle -0.5, -0.5, 1, -0.5, -0.5, 1\rangle$.
$\vec{v}_5 = \langle \sin(2\pi/3), \sin(4\pi/3), \sin(6\pi/3), \sin(8\pi/3), \sin(10\pi/3), \sin(12\pi/3)\rangle =$
$\langle 0.866, -0.866, 0, 0.866, -0.866, 0\rangle$.
$\vec{v}_6 = \langle \cos(3\pi/3), \cos(6\pi/3), \cos(9\pi/3), \cos(12\pi/3), \cos(15\pi/3), \cos(18\pi/3)\rangle = \langle -1, 1, -1, 1, -1, 1\rangle$.

These vectors are the $2K$ *real Fourier vectors.* The corresponding sinusoidal functions are called the $2K$ *real Fourier components*. These are the functions

$\mathbf{v}_1(t) = 1$.
For $J = 1 \ldots K$, $\mathbf{v}_{2J}(t) = \cos(J\pi t/T)$.
For $J = 1 \ldots K-1$, $\mathbf{v}_{2J+1}(t) = \sin(J\pi t/T)$.

Thus vector $\vec{v}_J$ is the $2K$ sample of function $\mathbf{v}_{2J}(t)$ over the interval $[0, T]$. (See figures 7.6 and 7.7.)

It is a fact that the $2K$ real Fourier vectors are linearly independent (in fact, orthogonal) and therefore form a basis for $\mathbb{R}^{2K}$, though we will not prove this. Therefore the sample vectors $\vec{a}$ and $\vec{g}$ can be written as linear sums over the Fourier vectors:

$\vec{a} = p_1 \cdot \vec{v}_1 + \ldots + p_{2K} \cdot \vec{v}_{2K}$
$\vec{g} = q_1 \cdot \vec{v}_1 + \ldots + q_{2K} \cdot \vec{v}_{2K}$

These coordinates are said to be in the *frequency domain.* The original coordinates are in the *time domain.*

It is reasonable to suppose that, if these equations hold for a dense sample with large K, then they approximately hold for the actual continuous functions involved. That is

$\mathbf{a} \approx p_1 \cdot \mathbf{v}_1 + \ldots + p_{2K} \cdot \mathbf{v}_{2K}$.
$\mathbf{g} \approx q_1 \cdot \mathbf{v}_1 + \ldots + q_{2K} \cdot \mathbf{v}_{2K}$

(There is a large theory of approximation, which discusses under what circumstances this is valid and how accurate you can expect the approximation to be.)

We now return to the signal processing function F that we introduced at the start of the section. It turns out that the function F does something rather simple with the Fourier vectors. Let us define the sequence of numbers $d_1 \ldots d_{2K}$ as follows:

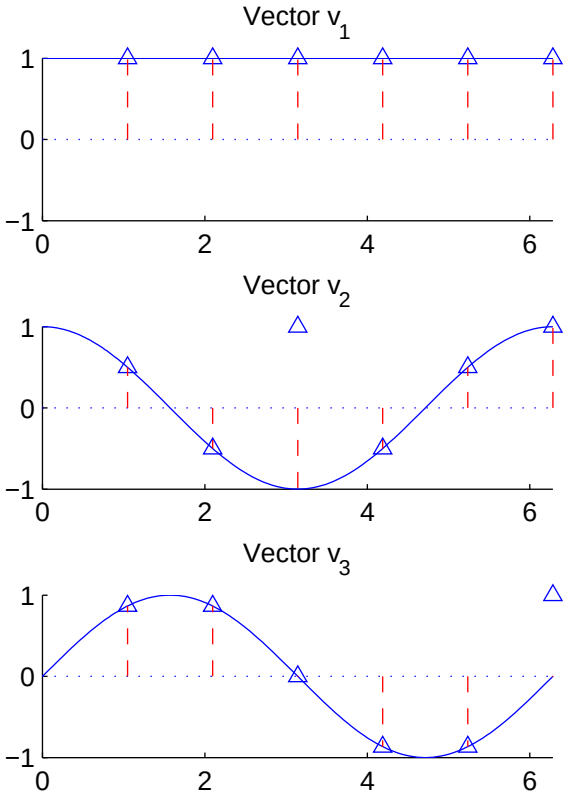


Figure 7.6: Discrete Fourier vectors as samplings of sine/cosine curves: $\vec{v}_1$, $\vec{v}_2$, and $\vec{v}_3$

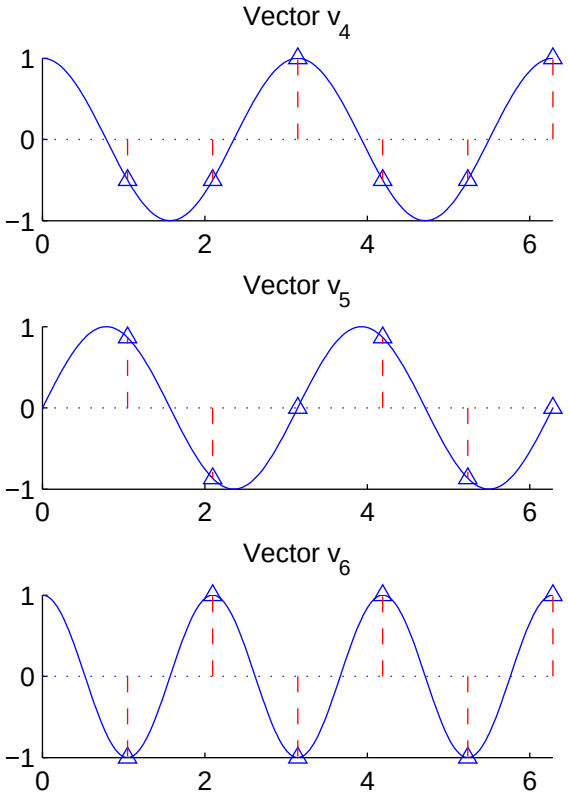


Figure 7.7: Discrete Fourier vectors as samplings of sine/cosine curves: $\vec{v}_4$, $\vec{v}_5$, and $\vec{v}_6$

$d_1 = A_1$.
For $J = 1 \ldots K$, $d_{2J} = A(\pi J/T)\cos(\delta(\pi J/T))$.
For $J = 1 \ldots K$, $d_{2J+1} = A(\pi J/T)\sin(\delta(\pi J/T))$

Then $F(\mathbf{v}_1) = d_1\mathbf{v}_1$

For $J = 1 \ldots K$,
$F(\mathbf{v}_{2J}) = F(\cos(\pi Jt/T)) =$
$A(\pi J/T)\cos(\pi J/T)\cos(\pi Jt/T) - A(\pi J/T)\sin(\pi J/T)\sin(\pi Jt/T) =$
$d_{2J}\mathbf{v}_{2J} - d_{2J+1}\mathbf{v}_{2J+1}$.

For $J = 1 \ldots K-1$,
$F(\mathbf{v}_{2J+1}) = F(\sin(\pi Jt/T)) =$
$A(\pi J/T)\cos(\pi J/T)\sin(\pi Jt/T) + A(\pi J/T)\sin(\pi J/T)\cos(\pi Jt/T) =$
$d_{2J+1}\mathbf{v}_j + d_{2J}\mathbf{v}_{J+1}$.

We can combine all this to get the following:

$$q_1\mathbf{v}_1 + \ldots + q_{2K}\mathbf{v}_{2K} \approx \mathbf{g} = F(\mathbf{a}) \approx F(p_1\mathbf{v}_1 + \ldots + p_{2K}\mathbf{v}_{2K}) =$$

$$p_1d_1\mathbf{v}_1 + p_2(d_2\mathbf{v}_2 - d_3\mathbf{v}_3) + p_3(d_2\mathbf{v}_3 + d_2\mathbf{v}_2) + p_4(d_4\mathbf{v}_4 - d_5\mathbf{v}_5) + p_5(d_5\mathbf{v}_5 + d_4\mathbf{v}_4) + \ldots + p_{2K}d_{2K}\mathbf{v}_{2K} =$$
$$d_1p_1\mathbf{v}_1 + (d_2p_2 + d_3p_3)\mathbf{v}_2 + (-d_3p_2 + d_2p_3)\mathbf{v}_3 + (d_4p_4 + d_5p_5)\mathbf{v}_4 + (-d_5p_4 + d_4p_5)\mathbf{v}_5 + \ldots + d_{2K}p_{2K}\mathbf{v}_{2K}$$

Comparing the coefficients of $\mathbf{v}_J$ in the first expression above and the last, and using the fact that the $\mathbf{v}_J$ are linearly independent, we conclude that

$q_1 = d_1p_1$.
$q_2 = d_2p_2 + d_3p_3$
$q_3 = -d_3p_2 + d_2p_3$
$q_4 = d_4p_4 + d_5p_5$
$q_5 = -d_5p_4 + d_4p_5$
$\ldots$
$q_{2K} = d_{2K}p_{2K}$

So $\vec{q}$ is a linear transformation of $\vec{p}$ with a matrix D that is nearly a diagonal:

$$\vec{q} = \begin{bmatrix} d_1 & 0 & 0 & 0 & 0 & \ldots & 0 \\ 0 & d_2 & d_3 & 0 & 0 & \ldots & 0 \\ 0 & -d_3 & d_2 & 0 & 0 & \ldots & 0 \\ 0 & 0 & 0 & d_4 & d_5 & \ldots & 0 \\ 0 & 0 & 0 & -d_5 & d_4 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & 0 & 0 & \ldots & d_{2K} \end{bmatrix} \cdot \vec{p}$$

D represents the signal processing characteristics of the device. It is a sparse matrix with $4K - 2$ non-zero elements. The multiplication $D \cdot \vec{p}$ can be carried out time $O(K)$. It is also easy to invert, if you want to go from output to input. D^{-1} is a matrix of the same structure, consisting of the inverse of each 1×1 or 2×2 square. So the inverse can be computed in time $O(K)$; it is again a sparse matrix, and multiplication by the inverse is carried out in time $O(K)$.

But of course this simple form only applies to vectors in the *frequency domain*, whereas we actually always start from vectors in the time domain, and generally we want to end there. That is where our theory of basis change comes in. Let M be the matrix whose columns are the Fourier vectors. Then

multiplication by M^{-1} transforms vectors in the time domain to vectors in the frequency domain, and multiplication by M transforms vectors in the frequency domain back into the time domain. So $\vec{g} = M \cdot D \cdot M^{-1} \cdot \vec{a}$.

That doesn't sound very promising — M and M^{-1} are large, non-sparse matrices. However, there are three facts that come to our rescue here:

- The Fourier matrix of size $2K$ depends only on K and not on the signal processor characteristics F and certainly not on the input $\vec{p}$. Therefore M and its inverse can be computed once and for all, and then reused for all processors and inputs.
- Since the columns of M are orthogonal, M^{-1} is just M^T with each row divided by its length squared.
- Multiplying a vector $\vec{v}$ by M and by M^{-1} does not require time $O(K^2)$; it requires only time $O(K \log K)$. The algorithm to achieve this is known as the Fast Fourier transform. In its modern form, it was discovered by Cooley and Tukey, but a version was known to Gauss. The explanation of this algorithm is beyond the scope of this book; see for example [Cormen et al., 2009].

The fast Fourier transform is executed by electronic devices all over the world millions of times every second. It is no exaggeration to say that modern electronic and communication depend critically on the fact that this basis transformation can be computed in time $O(K \log K)$ rather than time $O(K^2)$.

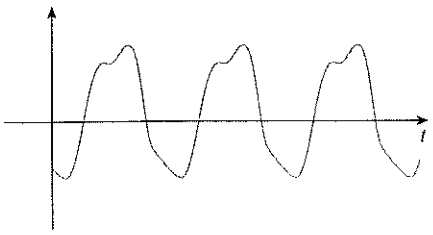
7.6.1 Other applications of the Fourier transform

There are many other applications of the Fourier transform. One important category of application is in the *recognition* of waveforms. For example figure 7.8 shows the waveform for a sustained D note on the flute and on the violin.[5] The two are obviously very different, but it is not immediately obvious how one would best distinguish them algorithmically. However, if one applies a Fourier transform, the distinction is easily made: the coefficients on higher frequency components (called "harmonics" in the context of musical notes) are much larger in the violin than in the flute. (This kind of analysis does not by any means account for all the recognizable differences in timbre between different musical instruments.) The plot in the lower diagram is the energy spectrum; that is, the square of the sum of the coefficients of the sine and cosine components at each frequency. (The energy spectrum does not contain enough information to reconstruct the signal, since it throws away the phase information.)

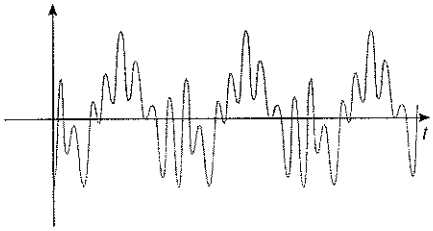
Another common application is in *denoising* a signal. In many situations, it can be assumed that the low frequency components of a waveform are the signal and the high frequency components are noise. A low-pass filter, which keeps only the low frequency components, can easily be constructed by performing a DFT, deleting the high-frequency components, and then translating back to the time domain. (Such filters can also be built out of analog components; but software is often easier to construct, modify, and integrate.)

There are innumerable other applications of the DFT, including image deblurring, image compression, recovering signals from samples, tomography, and finance (Marks 2009).

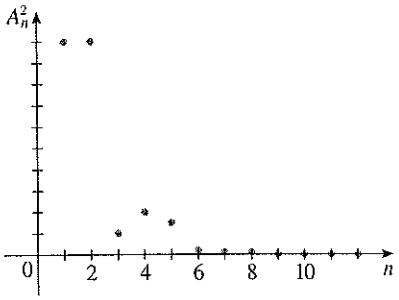
[5] James Stewart, *Essential Calculus: Early Transcendentals*, Cengage Learning, 2005. http://www.stewartcalculus.com



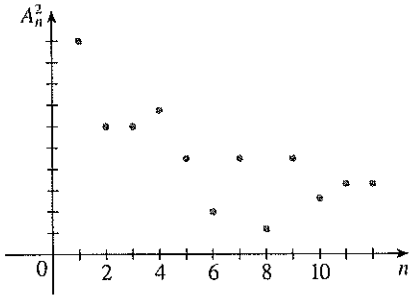
(a) Flute



(b) Violin



(a) Flute



(b) Violin

7.6.2 The complex Fourier transform

The discrete Fourier transform is generally presented using vectors and matrices whose components are complex numbers. In particular, code for computing the DFT, such as MATLAB's fft function, mostly use the complex version. The complex DFT is in many ways simpler than the real DFT presented above; however, explaining it would require a discussion of the theory of matrices over complex numbers. This theory has some important differences from matrices over the reals and it is beyond the scope of this book. In section 7.10 we give "black box" code to convert the complex "fft" function provided by MATLAB to the real DFT described above.

7.7 Singular value decomposition

In this section, we will show that *every* linear transformation takes a particularly simple form, with one particular choice of the basis in the domain and another in the range. This is known as the *singular value decomposition (SVD).* We will begin by defining the SVD, and then describe some of its properties and applications.

Theorem 7.4. *Let M be an $m \times n$ matrix. Let $r = \text{Rank}(M)$. Then there exists an orthonormal basis $\hat{b}_1 \dots \hat{b}_n$ for $\mathbb{R}^n$ such that $\{M \cdot \hat{b}_1 \dots M \cdot \hat{b}_r\}$ is an orthogonal basis for* Image(M).

In theorem 7.4 the vectors $\hat{b}_1 \dots \hat{b}_n$ are called the *right singular vectors* for M; these form an orthogonal basis for $\mathbb{R}^n$. The vectors $\hat{b}_{r+1} \dots \hat{b}_n$ are in Null(M) and are thus an orthonormal basis for Null(M). For $i = 1 \dots n$, let $\sigma_i = |M \cdot \hat{b}_i|$. The values $\sigma_1 \dots \sigma_n$ are called the *singular values* for M. Note that if $r < n$ then for $i = r+1 \dots n$, $\sigma_i = 0$. For $i = 1 \dots r$ let $\hat{c}_i = M \cdot \hat{b}_i / \sigma_i$. The vectors $\hat{c}_1 \dots \hat{c}_r$ are the *left singular vectors* for M. By theorem 7.4, $\hat{c}_1 \dots \hat{c}_r$ are an orthogonal basis for Image(M).

The proof of theorem 7.4 is not difficult; we give it at the end of the section.

The set of singular values is uniquely defined for any M. The set of singular vectors is not quite unique. If the value σ_i occurs only once in the list of singular values, then there are two choices for the associated vector; one is the negative of the other. If the same value occurs q times in the list of singular values, then there is a q-dimensional subspace of vectors associated with that value, and any orthonormal basis for that subspace will serve as the associated right singular vectors.

The SVD can be visualized as follows: Consider the n-dimensional sphere S of unit vectors in $\mathbb{R}^n$. Now consider $M \cdot S = \{M \cdot \hat{s} | \hat{s} \in S\}$. $M \cdot S$ is an *ellipsoid* within the subspace Image(M). The semi-axes of the ellipsoid are the values of $M \cdot \hat{b}_i$. So the lengths of the semi-axes are the singular values. The singular vectors $\hat{b}_i$ are the inverse image of the axes under M^{-1}.

The singular values and vectors can be defined using the following algorithm:

SVD Algorithm

$\mathcal{V} \leftarrow \mathbb{R}^n$; (1)
for $(i \leftarrow 1 \dots n)$ (2)
  $\hat{b}_i \leftarrow$ the unit vector $\hat{b}$ in $\mathcal{V}$ for which $|M \cdot \hat{b}|$ is maximal; (3)
  $\sigma_i \leftarrow |M \cdot \hat{b}_i|$. (4)
  if $\sigma_i \neq 0$ then $\hat{c}_i = M \cdot \vec{b}_i / \sigma_i$; (5)
  $\mathcal{V} \leftarrow$ the orthogonal complement of $\{\hat{b}\}$ in $\mathcal{V}$ (6)
endfor

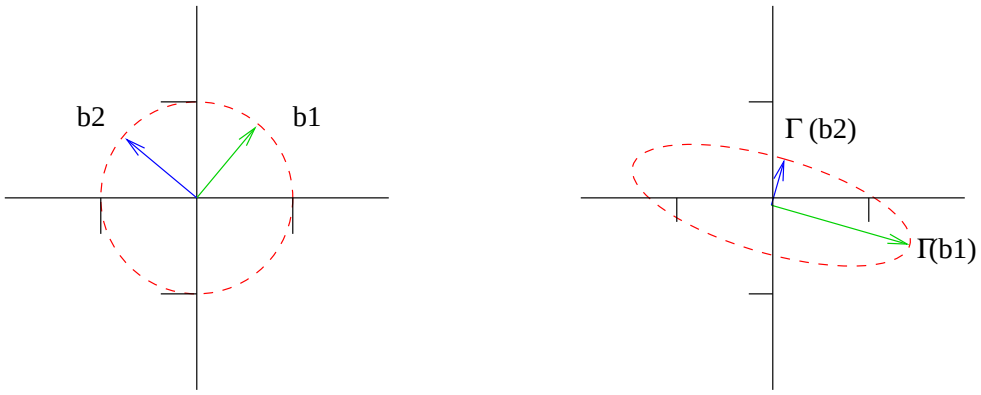


Figure 7.9: Example 7.1: SVD

That is: The first singular vector $\hat{b}_1$ is the unit vector $\hat{u}$ that maximizes $M\hat{u}$. The second singular vector $\hat{b}_2$ is the unit vector $\hat{u}$ orthogonal to $\hat{b}_1$ that maximizes $M\hat{u}$. The third singular vector $\hat{b}_3$ is the unit vector $\hat{u}$ orthogonal to both $\hat{b}_1$ and $\hat{b}_2$ that maximizes $M\hat{u}$. And so on.

Alternatively, you can go from smallest to largest. That is: The last singular vector $\hat{b}_n$ is the unit vector $\hat{u}$ that minimizes $M\hat{u}$. The second to last singular vector $\hat{b}_{n-1}$ is the unit vector $\hat{u}$ orthogonal to $\hat{b}_1$ that minimizes $M\hat{u}$. And so on. You end up with the same sets of singular values and singular vectors.

As an actual algorithm, this does not work very well, because calculating the maximum in step (3) is difficult; it involves the maximization of the quadratic function $(M\hat{b}) \cdot (M\hat{b})$ over the quadratic surface $\hat{b} \cdot \hat{b} = 1$, and over the cross-section of that surface with the linear subspace $\mathcal{V}$. The algorithms that are actually used in computing the SVD are beyond the scope of this book; see (Trefethen and Bau, 1997).

Example 7.1 (Figure 7.9): Let

$$M = \begin{bmatrix} .0752 & 1.236 \\ -0.636 & -0.048 \end{bmatrix}$$

and let $\hat{b}_1 = \langle 0.6, 0.8 \rangle$, $\hat{b}_2 = \langle -0.8, 0.6 \rangle$, $\hat{c}_1 = \langle 0.96, -0.28 \rangle$, and $\hat{c}_2 = \langle 0.28, 0.96 \rangle$.
It is easily checked that $\{\hat{b}_1, \hat{b}_2\}$ and $\{\hat{c}_1, \hat{c}_2\}$ are orthonormal bases, and that $M\hat{b}_1 = 1.5 \cdot \vec{c}_1$ and $M\hat{b}_2 = 0.5 \cdot \vec{c}_2$. Thus the right singular values are $\hat{b}_1$ and $\hat{b}_2$; the left singular values are $\hat{c}_1$ and $\hat{c}_2$; and the singular values are $\sigma_1 = 1.5$ and $\sigma_2 = 0.5$.

Example 7.2: Let

$$M = \begin{bmatrix} 1.0447 & -1.4777 & 0.9553 \\ 2.4761 & -2.2261 & 0.9880 \end{bmatrix}$$

and let $\hat{b}_1 = \langle 2/3, 2/3, 1/3 \rangle$, $\hat{b}_2 = \langle -2/3, 1/3, 2/3 \rangle$, $\hat{b}_3 = \langle 1/3, -2/3, 2/3 \rangle$;
$\hat{c}_1 = \langle 0.5, 0.866 \rangle$, and $\hat{c}_2 = \langle -0.866, 0.5 \rangle$,

It is easily checked that $\{\hat{b}_1, \hat{b}_2, \hat{b}_3\}$ and $\{\hat{c}_1, \hat{c}_2\}$ are orthonormal sets, and that $M\hat{b}_1 = 4\vec{c}_1$, $M\hat{b}_2 = 0.5\vec{c}_2$, and $M\hat{b}_3 = \vec{0}$. Thus $\hat{b}_1$, $\hat{b}_2$, and $\hat{b}_3$ are the right singular vectors; $\hat{c}_1$, $\hat{c}_2$ are the left singular vectors, and $\sigma_1 = 4, \sigma_2 = 0.5, \sigma_3 = 0$ are the singular values.

7.7.1 Matrix decomposition

Let M be an $m \times n$ matrix with rank r. Let $\sigma_1 \dots \sigma_n$ be the singular values of M, let $\mathcal{B} = \{\hat{b}_1 \dots \hat{b}_n\}$ be the corresponding right singular vectors; and let $\{\hat{c}_1 \dots \hat{c}_r\}$ be the left singular vectors. If $r < m$, then let $\hat{c}_{r+1} \dots \hat{c}_m$ be an orthonormal basis for the orthogonal complement to Image(M) in $\mathbb{R}^m$; thus $\mathcal{C} = \{\hat{c}_1 \dots \hat{c}_m\}$ is an orthonormal basis for $\mathbb{R}^m$.

Now, let $\vec{v}$ be any vector in $\mathbb{R}^n$. Let $p_1 \dots p_n$ be the coordinates of $\vec{v}$ in $\mathcal{B}$. Thus $\vec{v} = p_1 \cdot \hat{b}_1 + \ldots + p_n \hat{b}_n$. So

$$M \cdot \vec{v} = M \cdot (p_1 \cdot \hat{b}_1 + \ldots + p_n \hat{b}_n) = p_1 M \cdot \hat{b}_1 + \ldots + p_n M \cdot \hat{b}_n = p_1 \sigma_1 \hat{c}_1 + \ldots + p_r \sigma_r \hat{c}_r$$

In the last step above, the terms after r are all zero, and can be dropped.

Thus, the coordinates of $M\vec{v}$ with respect to $\mathcal{C}$ are $\langle p_1\sigma_1, p_2\sigma_2 \dots p_r\sigma_r, 0, 0 \ldots \rangle$, filled out at the end with $m - r$ 0's.

Therefore we have $\text{Coords}(M\vec{v}, \mathcal{C}) = S \cdot \text{Coords}(\vec{v}, \mathcal{B})$, where S is the $m \times n$ diagonal matrix with the singular values on the diagonal.

Let B be the $n \times n$ matrix with columns $\hat{b}_1 \dots \hat{b}_n$ and let L be the $m \times m$ matrix with columns $\hat{c}_1 \dots \hat{c}_m$. By theorem 7.2 we have $\text{Coords}(\vec{v}, \mathcal{B}) = B^{-1}\vec{v}$ and $M \cdot \vec{v} = L \cdot \text{Coords}(M \cdot \vec{v}, \mathcal{C})$. Let $R = B^{-1}$; since B is an orthonormal matrix $R = B^T$. Putting this together we have $M\vec{v} = (L \cdot S \cdot R)\vec{v}$. Since L, S, and R are independent of the choice of $\vec{v}$, this equation holds for all $\vec{v}$ so we must have $M = L \cdot S \cdot R$. We have thus proven the following theorem.

Theorem 7.5. *Let M be any $m \times n$ matrix. Then there exists matrices L, S, R such that:*

- *S is a diagonal matrix with elements on the diagonal in descending order.*
- *R is an $n \times n$ orthonormal matrix,*
- *L is an $m \times m$ orthonormal matrix.*
- *$M = L \cdot S \cdot R$.*

Specifically the diagonal elements of S are the singular values of M; the rows of R are the right singular vectors, and the columns of L are the left singular vectors.

The expression of M as the product $L \cdot S \cdot R$ is known as the *singular value decomposition* of M. Strictly speaking, this is a slight misnomer, since the decomposition is not unique, in the case where the same singular value appears multiply in S. In that case, the theorems below apply to all the singular value decompositions of M.

For instance, in example 7.1, we have

$$\begin{bmatrix} .0752 & 1.236 \\ -0.636 & -0.048 \end{bmatrix} = \begin{bmatrix} 0.96 & 0.28 \\ -0.28 & 0.96 \end{bmatrix} \cdot \begin{bmatrix} 1.5 & 0 \\ 0 & 0.5 \end{bmatrix} \cdot \begin{bmatrix} 0.6 & 0.8 \\ -0.8 & 0.6 \end{bmatrix}$$

In example 7.2 we have

$$\begin{bmatrix} 1.0447 & -1.4777 & 0.9553 \\ 2.4761 & -2.2261 & 0.9880 \end{bmatrix} = \begin{bmatrix} 0.5 & -0.8660 \\ 0.8660 & 0.5 \end{bmatrix} \cdot \begin{bmatrix} 4.0 & 0 & 0 \\ 0 & 0.5 & 0 \end{bmatrix} \cdot \begin{bmatrix} 0.6667 & -0.6667 & 0.3333 \\ -0.6667 & 0.3333 & 0.6667 \\ 0.3333 & 0.6667 & 0.6667 \end{bmatrix}$$

Now consider any $n \times n$ non-singular matrix M. Then Rank$(M) = n$, so all the singular values $\sigma_1 \ldots \sigma_n$ are non-zero. Let $\vec{b}_1 \ldots \vec{b}_n$ be the right singular vectors, and let $\vec{c}_1 \ldots \vec{c}_n$ be the left singular vectors; Thus $M\vec{b}_i = \sigma_i \vec{c}_i$. Therefore $M^{-1}\vec{c}_i = (1/\sigma_i)\vec{b}_i$. Therefore, the left singular vectors of M are the right singular vectors of M^{-1} and vice versa; the singular values of M^{-1} are the reciprocals of the singular values of M. (If you want to get the singular values in descending order, then of course you have to reverse all of the numberings.)

Note that if we start with the SVD decomposition equation $M = LSR$ and we take the transpose of both sides, we get

$$M^T = (LSR)^T = R^T S^T L^T$$

But since L and R are orthnormal matrices, their transposes are likewise orthonormal; and since S is a diagonal matrix, $S^T = S$. Therefore the above equation is the SVD decomposition for M^T. In particular, the singular values of M^T are the same as those for M; as with most theorems about the transpose, this is not at all obvious from the fundamental definition.

7.7.2 Proof of theorem 7.4 (Optional)

We begin with a lemma:

Lemma 7.6. *Let M be a matrix. Let $\hat{p}$ and $\hat{q}$ be orthogonal unit vectors. Let $\vec{u} = M \cdot \hat{p}$ and let $\vec{v} = M \cdot \hat{q}$. If $\vec{u} \bullet \vec{v} > 0$ then there exists a unit vector $\hat{w}$ which is a linear sum of $\hat{p}$ and $\hat{q}$ such that $|M\hat{w}| > |M\hat{p}|$.*

Proof: We will choose $\hat{w}$ to be the unit vector parallel to $\hat{p} + \epsilon\hat{q}$ where $\epsilon > 0$ is a value we will specify later. Thus $\vec{e} = \hat{p} + \epsilon\hat{q}$ and $\vec{w} = \vec{e}/|\vec{e}|$. Since $\hat{p}$ and $\hat{q}$ are orthogonal, $|\vec{e}| = \sqrt{1+\epsilon^2}$, so $1/|\vec{e}|^2 = 1/(1+\epsilon^2) > 1 - \epsilon^2$. Now $M \cdot \hat{w} = M \cdot ((\hat{p} + \epsilon\hat{q})/|\vec{e}|) = (\vec{u} + \epsilon\vec{v})/|\vec{e}|$ so

$$(|M\hat{w}|)^2 = (M\hat{w}) \bullet (M\hat{w}) = (\vec{u} \bullet \vec{u} + 2\epsilon\vec{u} \bullet \vec{v} + \epsilon^2 \vec{v} \bullet \vec{v})/|\vec{e}|^2 > (\vec{u} \bullet \vec{u} + 2\epsilon\vec{u} \bullet \vec{v} + \epsilon^2 \vec{v} \bullet \vec{v})(1 - \epsilon^2) =$$

$$|\vec{u}|^2 + 2\epsilon\vec{u} \bullet \vec{v} \pm O(\epsilon^2)$$

So as long as $\epsilon \ll \vec{u} \bullet \vec{v}$, we have $|M \cdot \hat{w}|^2 > |\vec{u}|^2 = |M \cdot \hat{p}|^2$, so $|M \cdot \hat{w}| > |M \cdot \hat{p}|$. ∎

Corollary 7.7. *Let M be an $m \times n$ matrix and let $\mathcal{V}$ be a subspace of $\mathbb{R}^n$. Let $\hat{p}$ be a unit vector in $\mathcal{V}$ such that $|M \cdot \hat{p}|$ is maximal, and let $\hat{z}$ be a unit vector in $\mathcal{V}$ which is orthogonal to $\hat{p}$. Then $M \cdot \hat{z}$ is orthogonal to $M \cdot \hat{p}$.*

Proof of the contrapositive. Suppose that $M\hat{z}$ is not orthogonal to $M\hat{p}$; thus $(M\hat{z}) \bullet (M\hat{p}) \neq 0$. If $(M\hat{z}) \bullet (M\hat{p}) < 0$ then let $\hat{q} = -\hat{z}$; else let $\hat{q} = \hat{z}$. Then $(M\hat{q}) \bullet (M\hat{p}) > 0$. By lemma 7.6, there exists a unit vector $\hat{w}$ in $\mathcal{V}$ such that $|M\hat{w}| > |M\hat{p}|$. But then $\hat{p}$ is not the unit vector in $\mathcal{V}$ that maximizes $|M\hat{p}|$. ∎

We now turn to the proof of theorem 7.4. We prove that theorem 7.4 is true by proving that the SVD algorithm computes sets of right and left singular vectors and singular values that satisfy the theorem. This proof has three parts.

Part I: The algorithm can always be executed. The only part of the algorithm that is at all difficult in that regard is in step (3), the existence of a unit vector in $\mathcal{V}$ that maximizes $|M \cdot \hat{b}|$. The existence of such a maximal value follows from a basic, general theorem of real analysis that a continuous function over a closed, bounded set has a maximal value (this theory is beyond the scope of this book); here the function $|M \cdot \hat{b}|$ is the continuous function and the set of unit vectors in the vector space $\mathcal{V}$ is closed and bounded. Since the dimension of $\mathcal{V}$ is reduced by 1 at each iteration of the for loop, it works its way down from $\mathbb{R}^n$ at the start of the algorithm to the zero space at the end; therefore, the algorithm terminates..

Part II: The vectors $\hat{b}_1 \ldots \hat{b}_n$ are orthogonal, since at the end of the ith iteration $\mathcal{V}$ is the orthogonal complement to $\hat{b}_1 \ldots \hat{b}_i$, and all the remaining values of $\hat{b}$ are chosen from within this space.

Part III: All that remains to be shown is that the vectors $\hat{c}_1 \ldots \hat{c}_r$ are orthogonal. Consider any two indices $i < j$. On the ith iteration of the loop, $\hat{b}_i$ is the unit vector in the current value of $\mathcal{V}$ that maximizes $|M \cdot \hat{b}_i|$. Since $\hat{b}_j$ is in that value of $\mathcal{V}$ and since $\hat{b}_j$ and $\hat{b}_i$ are orthogonal, it follows from corollary 7.7 that $M\hat{b}_i$ and $M\hat{b}_j$ are orthogonal, so $\hat{c}_i$ and $\hat{c}_j$ are orthogonal.

7.8 Further properties of the SVD

The SVD can be used to solve many other important minimization and maximization problems associated with a matrix or a linear transformation. We mention, without proof, some of the most important of these. What is remarkable is that all these different problems have such closely related solutions.

Definition 7.1. *Let A and B be two $m \times n$ matrices. The* Frobenius distance *between A and B, denoted $d_2(A, B)$ is defined as*

$$d_2(A, B) = \sqrt{\sum_{i,j} (A[i, j] - B[i, j])^2}$$

The absolute distance *between A and B, denoted $d_1(A, B)$ is defined as*

$$d_1(A, B) = \sum_{i,j} |A[i, j] - B[i, j]|$$

If you flatten A and B out to be two long, $m \cdot n$ dimensional vectors, then the Frobenius distance is just the Euclidean distance between these vectors.

Example 7.3

$$\text{Let } A = \begin{bmatrix} 1 & 5 & 2 \\ 8 & 2 & 3 \end{bmatrix} \text{ and } B = \begin{bmatrix} 2 & 8 & 2 \\ 6 & 4 & 2 \end{bmatrix}$$

$$\text{Then } d_2(A, B) = \sqrt{(1-2)^2 + (5-8)^2 + (2-2)^2 + (8-6)^2 + (2-4)^2 + (3-2)^2} = \sqrt{19} = 4.3589$$

$$d_1(A, B) = |1-2| + |5-8| + |2-2| + |8-6| + |2-4| + |3-2| = 9$$

Definition 7.2. *Let A be an $m \times n$ matrix; let $k \leq \min(m, n)$ and let L, S, R be the SVD decomposition of A; thus $A = L \cdot S \cdot R$. Let S^k be the diagonal matrix whose first k diagonal elements are equal to the corresponding element of S and whose remaining elements are 0. Let L^k be the $m \times m$ matrix in which the first k columns are equal to L and the rest are 0. Let R^k be the $n \times n$ matrix in which the first k rows are equal to L and the rest are 0. Then the* kth SVD reconstruction *of A is the product $LS^kR = L^kS^kR^k$.*

Theorem 7.8. *Let A be an $m \times n$ matrix. The matrix of rank k that is closest to A is the kth SVD reconstruction of A, when "closeness" is measured, either by the Frobenius distance, or by the absolute distance.*

Moreover, if the singular values that are dropped in S^k are small as compared to those that are included, then these two distances are small as compared to the inherent size of A. For details see (Trefethen and Bau, 1997).

In section 7.9.3, we will discuss how this theorem can be applied to data compression.

Example 7.3

```
>> A=[1,0,1,0; 2,4,6,7; 3,8,10,2]
A =
     1     0     1     0
     2     4     6     7
     3     8    10     2

>> [L,S,R]=svd(A)        % SVD Decomposition
L =
   -0.0590    0.0532   -0.9968
   -0.5878   -0.8090   -0.0084
   -0.8069    0.5854    0.0790
S =
   16.1103         0         0         0
         0    4.8394         0         0
         0         0    1.0185         0
R =
   -0.2269    0.0396   -0.7626   -0.6045
   -0.5466    0.2991    0.5875   -0.5163
   -0.7234    0.2178   -0.2527    0.6045
   -0.3556   -0.9282    0.0975   -0.0504

>> R=R';
>> L*S*R
ans =
    1.0000    0.0000    1.0000    0.0000
    2.0000    4.0000    6.0000    7.0000
    3.0000    8.0000   10.0000    2.0000

>> S1=zeros(3,4);
>> S1(1,1)=S(1,1)
S1 =
   16.1103         0         0         0
         0         0         0         0
         0         0         0         0

>> A1=L*S1*R                    % First SVD Approximation
A1 =
    0.2156    0.5194    0.6874    0.3379
    2.1485    5.1762    6.8504    3.3671
    2.9492    7.1052    9.4034    4.6219
>> rank(A1)
ans =
    1
>> norm(A1-A)                   % Frobenius distance
ans =
    4.8394
>> sum(sum(abs(A1-A)))          % Absolute distance
ans =
   11.9264
```

```
>> S2(2,2)=S(2,2)
S2 =
   16.1103         0         0         0
         0    4.8394         0         0
         0         0         0         0
>> A2=L*S2*R                      % Second SVD Approximation
A2 =
    0.2258    0.5964    0.7435    0.0990
    1.9935    4.0050    5.9978    7.0008
    3.0613    7.9527   10.0203    1.9922
>> rank(A2)
ans =
    2
>> norm(A2-A)                     % Frobenius distance
ans =
    1.0185
>> sum(sum(abs(A2-A)))            % Absolute distance
ans =
    1.8774
```

We have seen that the first right singular vector for matrix A is the unit vector $\hat{u}$ such that $|A \cdot \hat{u}|$ is maximal; and that the last right singular vector is the vector $\hat{u}$ for which $|A \cdot \hat{u}|$ is minimal. The next two theorems state that this generalizes to the first and last k singular vectors as a collection in two different ways.

Theorem 7.9. *Let A be an $m \times n$ matrix and let $k \leq n$. For any orthonormal set $\{\hat{u}_1 \dots \hat{u}_k\}$ of K n-dimensional unit vectors, consider the sum $\sum_{i=1}^{k} |A \cdot \hat{u}_i|^2$. The set of k orthonormal vectors that maximizes this sum is the set of the first k right singular vectors of A. The set of k orthonormal vectors that minimizes this sum is the set of the last k right singular vectors of A.*

In section 14.6, we will discuss an application of this theorem to statistical analysis.

The final theorem states that the space spanned by the k first right singular vectors of a linear transformation Γ is the k-dimensional subspace of $\mathbb{R}^n$ that is most expanded by Γ, and that the space spanned by the last k span is the space that is least expanded.

First we need to define the amount that a linear transformation expands or contracts a subspace; this is done using the determinant.

Definition 7.3. *Let Γ be a linear transformation from $\mathbb{R}^n$ to $\mathbb{R}^m$. Let $k \leq \text{Rank}(\Gamma)$. Let $\mathcal{V}$ be any k-dimensional subspace of $\mathbb{R}^n$ such that $\mathcal{V} \cap \text{Null}(\Gamma) = \{\vec{0}\}$. Let $\mathcal{B} = \langle \hat{v}_1 \dots \hat{v}_k \rangle$ be an orthonormal basis for $\mathcal{V}$ and let $\mathcal{C} = \langle \hat{u}_1 \dots \hat{u}_k \rangle$ be an orthonormal basis for $\Gamma(\mathcal{V})$. Let G be the matrix such that, for any vector $\vec{v} \in \mathcal{V}$, $\text{Coords}(\Gamma(\vec{v}), \mathcal{C}) = G \cdot \text{Coords}(\vec{v}, \mathcal{B})$. Then the* determinant of Γ restricted to $\mathcal{V}$ *denoted $\text{Det}_{\mathcal{V}}(\Gamma)$ is defined as $|\text{Det}(G)|$.*

In definition 7.3, the value $\text{Det}_{\mathcal{V}}(\Gamma)$ does not depend on the choice of the bases $\mathcal{B}$ and $\mathcal{C}$. The geometric significance of this quantity is given in the following theorem.

Theorem 7.10. *Let Γ, k, and $\mathcal{V}$ be as in definition 7.3. Let $\mathbf{R}$ be a region in $\mathcal{V}$. Then the k-dimensional measure (i.e. the k-dimensional analogue of area or volume) of $\Gamma(\mathbf{R})$ is equal to $\text{Det}_{\mathcal{V}}(\Gamma)$ times the k-dimensional measure of $\mathbf{R}$.*

The determinant restricted to $\mathcal{V}$ is thus a measure of how much Γ expands or contracts regions in $\mathcal{V}$.

We can now relate maximal and minimal expansion to the singular vectors.

Theorem 7.11. *Let A be an $m \times n$ matrix, and let Γ be the corresponding linear transformation from $\mathbb{R}^n$ to $\mathbb{R}^m$. Let $r = \text{Rank}(\Gamma)$ and let $k < r$.*

- *Over all k-dimensional subspaces $\mathcal{V}$ such that $\mathcal{V} \cap \text{Null}(\Gamma) = \{\vec{0}\}$, the maximum value of $\text{Det}_{\mathcal{V}}(\Gamma)$ is achieved when $\mathcal{V}$ is the subspace spanned by the k first right singular vectors of A.*
- *Over all k-dimensional subspaces $\mathcal{V}$ such that $\mathcal{V}$ is orthogonal to $\text{Null}(\Gamma)$, the minimum value of $\text{Det}_{\mathcal{V}}(\Gamma)$ is achieved when $\mathcal{V}$ is the subspace spanned by the k last singular vectors of A with non-zero singular value; that is, the vectors $\hat{u}_{r+1-k} \ldots \hat{u}_r$, where $\hat{u}_1, \hat{u}_2 \ldots \hat{u}_n$ are the right singular vectors.*

7.8.1 Eigenvalues of a symmetric matrix

The theory of eigenvalues and eigenvectors is a very important aspect of matrix theory for applications in physics and engineering, as well as purely mathematical analysis. We have largely omitted it in this textbook, first because it is much less important in computer science applications, and second because an adequate general discussion necessarily involves linear algebra over the field of complex numbers. However, for the particular case of a symmetric matrix, only real numbers are involved, and the theory is closely related (in fact, identical) to the theory of singular values, so we describe that briefly here.

Definition 7.4. *Let A be an $n \times n$ matrix. An n-dimensional vector $\vec{v}$ is an* eigenvector *of A with associated* eigenvalue *λ if $A \cdot \vec{v} = \lambda \cdot \vec{v}$.*

Definition 7.5. *A square matrix A is* symmetric *if $A^T = A$.*

Theorem 7.12. *Let A be a symmetric matrix. Let $\hat{r}$ be a right singular vector with corresponding singular value σ and corresponding left singular vector $\hat{l}$. Then $\hat{r}$ is an eigenvector with eigenvalue $\pm\sigma$ and thus $\hat{l} = \pm\hat{r}$.*

The proof is omitted. The converse — if the right singular vectors are eigenvectors then the matrix is symmetric — is easy (problem 7.4).

Corollary 7.13. *Let A be a symmetric $n \times n$ matrix. Then there exist n linearly independent real eigenvectors of A, with real eigenvalues. Moreover, the eigenvectors are all orthogonal.*

The significance of this corollary within the general theory of eigenvalues, is that for non-symmetric matrices, eigenvalues and eigenvectors may be complex, eigenvectors may not be orthogonal, and there may not exist n linearly independent eigenvectors even if complex vectors are considered. Thus, real symmetric matrices have eigenvectors that are strikingly well-behaved.

7.9 Applications of the SVD

In this section we discuss three applications of the SVD; condition number, approximate rank, and lossy compression. In section 14.6 we will discuss *principal component analysis*, which is an application of the SVD to statistics.

7.9.1 Condition number

The *condition number* of a function is a measure of how errors in the input propagate to become errors in the output; specifically, they are the ratio between the relative error in the output and the relative error in the input. For instance, suppose that you want to calculate $f(x)$, and you have an estimate $\tilde{x}$ of x that is accurate to within 1% of $|x|$; that is $|\tilde{x} - x| \leq .01x$. If the condition number of f is 4, then $f(\tilde{x})$ is within 4% of $f(x)$. If the condition number of f is 10, then $f(\tilde{x})$ is within 10% of $f(x)$. If the condition number of f is 1000, then $|f(\tilde{x}) - f(x)|$ may be 10 times as large as $|f(x)|$; in that case $f(\tilde{x})$ is useless as an estimate for most purposes.

Symbolically,

$$\text{Condition}(f) = \sup_{x,\tilde{x}} \frac{|f(\tilde{x}) - f(x)|/|f(x)|}{|\tilde{x} - x|/|x|}$$

where x and $\tilde{x}$ range over all values where none of the denominators involved are 0.

For a linear transformation, the condition number can be directly computed from the singular values.

Theorem 7.14. *If f is the linear transformation corresponding to matrix M, then the condition number of f is the ratio of the largest and smallest singular values: Condition$(f) = \sigma_1(M)/\sigma_n(M)$.*

It is easy to show that the condition number is at least as large as σ_1/σ_n. Let $\hat{b}_1$ and $\hat{b}_n$ be the right singular vectors corresponding to σ_1 and σ_n. Let $x = \hat{b}_n$ and let $\tilde{x} = \vec{b_n} + \epsilon\hat{b}_1$. Then $|x| = 1$; $|\tilde{x} - x| = \epsilon$, $|f(x)| = |f(\hat{b}_n)| = \sigma_n$ and $|f(\tilde{x}) - f(x)| = f(\tilde{x} - x) = f(\epsilon\hat{b}_1) = \epsilon\sigma_1$. So Condition$(f) \geq (\epsilon\sigma_1/\sigma_n)/(\epsilon/1) = \sigma_1/\sigma_n$.

Showing that the condition number is not larger than σ_1/σ_n takes a little more work, and we omit it here.

We can use this to gain more insight into the problems in section 5.5 that gave MATLAB such grief. Recalling the first example, let $d = 10^{-9}$ and let M be the matrix

$$M = \begin{bmatrix} 1+d & 1 \\ 1 & 1-d \end{bmatrix}$$

It is easily shown that the singular vectors are approximately $\langle\sqrt{1/2}, \sqrt{1/2}\rangle$ with singular value 2 and $\langle\sqrt{1/2}, -\sqrt{1/2}\rangle$ with singular value d. Hence, the condition number is $2/d = 2 \cdot 10^9$, so this is very ill-conditioned. In solving the linear equation $M\vec{x} = \langle 1, 1\rangle$, note that the singular values of M^{-1} are $10^9, 1/2$, and the condition number is again $2 \cdot 10^9$.

Another example is discussed in exercise 7.2

7.9.2 Computing rank in the presence of round-off

As discussed in section 5.2, the rank of matrix M can be computed by using Gaussian elimination to reduce M to row-echelon form and then counting the number of non-zero rows. This works very well when the coefficients of M are known exactly, and when the Gausssian elimination algorithm can be carried out precisely. However, if there is any noise in the coefficients of M, or any round-off error in the execution of Gaussian elimination, then Gaussian elimination does not give any useful information about the rank. For example, it does not work to discard any rows that are "close to" $\vec{0}$; Gaussian elimination normalizes the first coefficient in each row to 1, so no non-zero row is close to $\vec{0}$.

In this situation, the following method works well; it is, in fact, the method that MATLAB uses to compute rank. You set a small threshhold, you compute the singular values of M, and you conjecture

that singular values below the threshhold are actually zero, and that therefore the rank is equal to the number of singular values above the threshhold. This conjecture is reasonable in two senses. First, it often does give the true rank of M; it is indeed often the case that the singular values that are computed as small are actually zero, and appear as non-zero only because of round-off error. Second, even if the small singular values are actually non-zero, the rank r computed by this procedure is "nearly" right, in the sense that M is very close to a matrix M' of rank r; namely, the rth SVD reconstruction of M.

Choosing a suitable threshhold is a process of some delicacy; the right choice depends the size of M and on how M was constructed. The comments on assignment 6.1 discuss a case where MATLAB's default threshhold turns out to be too small.

7.9.3 Lossy compression

A *compression* algorithm Φ is one that takes as input a body of data D and constructs a representation $E = \Phi(D)$ such that

- The computer memory needed to record E is much less than the natural encoding of D.
- There is a decompression algorithm Ψ to reconstruct D from E. If $\Psi(E)$ is exactly equal to D then Φ is a *lossless* compression algorithm, If $\Psi(E)$ is approximately equal to D, then Φ is a *lossy* compression algorithm.

Whether a lossless compression algorithm is needed or whether a lossy compression algorithm will suffice depends on the application. For compressing text or computer programs, one needs lossless compression; reconstituting a text or program with each character code off by 1 bit is not acceptable. For pictures, sound, or video, however, lossy compression may merely result in a loss of quality, but still be usable; if every pixel in an image is within 1% of its true grey level, a human viewer will barely notice the difference.

SVD can be used for lossy compression as follows. Suppose that your data is encoded in a matrix $m \times n$ matrix M. Compute the SVD decomposition $M = LSR$. Choose a value k which is substantially less than m or n. Now let S' be the diagonal matrix with the first k singular values. Let R' be the matrix whose first k rows are the same as R and the rest are 0. Let L' be the matrix whose first k columns are the same as L and the rest are 0. Let $M' = L'S'R'$. By theorem 7.8, M' closely approximates M, particularly if the singular values that have been dropped are small compared to those that have been retained.

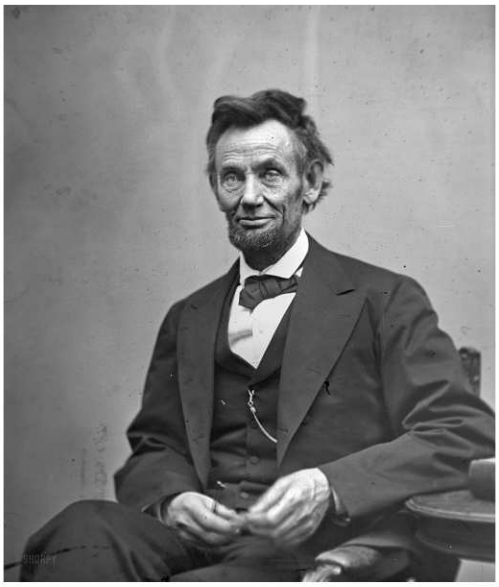
The compressed encoding here is to record the non-zero elements of L', S' and R'. L' has km non-zero elements, S' has k, and R' has kn, for a total of $k(m + n + 1)$; if k is small, then this is substantially smaller than the mn non-zero elements in M.

Figures 7.10 and 7.11 shows a gray-scale image and a line drawing, and and a few of their approximations with different values of k.

7.10 MATLAB

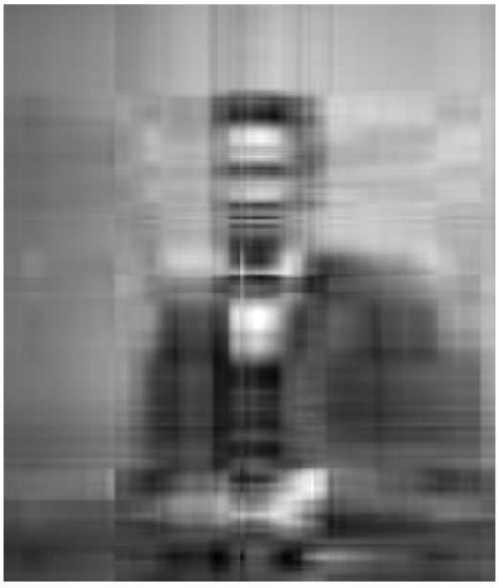
7.10.1 SVD in MATLAB

The MATLAB function `svd(M)` can be used in two ways. If you request one value to be returned then it returns the vector of singular values. If you request three values to be returned, then it returns the three matrices L, S, R.



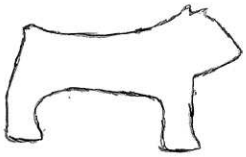
Original gray scale image

Reconstruction with 2 singular values

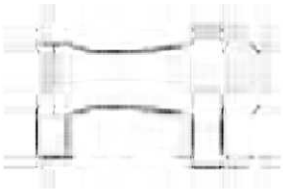


Reconstruction with 5 singular values

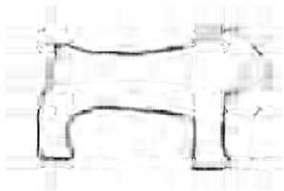
Reconstruction with 30 singular values



Original line drawing
of a bear
(after James Thurber)



Reconstruction from 5 singular values



Reconstruction from 10 singular values

```
% Example 7.2 in the text
>> M=[1.0447, -1.4777, 0.9553; 2.4761, -2.2261, 0.9880]
M =
    1.0447   -1.4777    0.9553
    2.4761   -2.2261    0.9880

>> svd(M)
ans =
    4.0000
    0.5000

>> [L,S,R]=svd(M)
L =
   -0.5000   -0.8660
   -0.8660    0.5000
S =
    4.0000         0         0
         0    0.5000         0
R =
   -0.6667    0.6667    0.3333
    0.6667    0.3334    0.6667
   -0.3333   -0.6667    0.6667

>> P=L*S*R'
ans =
    1.0447   -1.4777    0.9553
    2.4761   -2.2261    0.9880

>> norm(P-M)
ans =
   9.4928e-16
```

7.10.2 DFT in MATLAB

MATLAB provides built-in functions `fft` and `ifft` for carrying out the Fast Fourier Transform; however, these use the complex version of the FFT.

If you want to use the real DFT, as described in section 7.6, then there are two choices. The conceptually easy way is to use the function `trigBasis(K)` given below to construct the $2K \times 2K$ matrix M of Fourier component vectors. Then `M\V` will convert a vector `V` in the real domain to the frequency domain, and `M*V` will convert `V` from the frequency domain to the time domain. However, this loses the efficiency of the FFT.

To take advantage of the efficient FFT, I have provided two "black box" routines provided below that compute the real DFT using MATLAB's built-in FFT as a subroutine. The function `dft(V)` maps a column vector V from the time domain to the frequency domain; that is, `dft(V) = trigBasis(K)\V`. The function `idft(V)` maps a column vector V from the frequency domain to the time domain; that is `trigBasis(K) * V = idft(V)`.

If you are using the FFT, you should note that the algorithm works best if the dimension is a power of two or factorizable into small primes. It runs considerably slower if the dimension is a large prime, or has a large prime factor. Of course, depending on the application, you may not have any choice

about the dimension.

```
% File trigBasis.m
% Returns the matrix whose columns are the trigonometric Fourier components
% of size 2K
%
%      1  cos(pi/K)   sin(pi/K)   cos(2 pi/K) sin(2 pi/K) ... cos(pi)
%      1  cos(2 pi/K) sin(2 pi/K) cos(4 pi/K) sin(4 pi/K) ... cos(pi)
%      1  cos(3 pi/K) sin(3 pi/K) cos(6 pi/K) sin(6 pi/K) ... cos(pi)
%      ...


function b = trigBasis(K)
   N=2*K;
   b=zeros(N,N);
   b(:,1) = ones(N,1);
   for j=1:K
     for i=1:N
       b(i,2*j) = cos(i*j*pi/K);
       if (2*j ~= N) b(i,2*j+1) = sin(i*j*pi/K); end
     end
   end
end


% Example
>> trigBasis(2)
ans =
    1.0000    0.0000    1.0000   -1.0000
    1.0000   -1.0000    0.0000    1.0000
    1.0000   -0.0000   -1.0000   -1.0000
    1.0000    1.0000   -0.0000    1.0000
>> trigBasis(3)
ans =
    1.0000    0.5000    0.8660   -0.5000    0.8660   -1.0000
    1.0000   -0.5000    0.8660   -0.5000   -0.8660    1.0000
    1.0000   -1.0000    0.0000    1.0000   -0.0000   -1.0000
    1.0000   -0.5000   -0.8660   -0.5000    0.8660    1.0000
    1.0000    0.5000   -0.8660   -0.5000   -0.8660   -1.0000
    1.0000    1.0000   -0.0000    1.0000   -0.0000    1.0000

% File dft.m
% Converts column vector in time domain to vector in frequency domain.
%    using the real Fourier components discussed in the text
% Let X = < x[1] ... x[n] >
% Let F = dft(X)
% Then X[i] = F[1] + F[2] cos(pi i/N) + F[3] sin(pi i/N) +
%       ... F[N-2] cos(pi (N-1)/N) +F[N-1] sin(pi i (N-1)/N)) + F[N] cos(pi i).

% dft(x) is equal to trigBasis(N/2)\x but computes faster, since it uses
```

```
% the FFT.

function f = dft(x)
   n = size(x);
   n = n(1);
   y(1,1) = x(n,1);
   y(2:n,1) = x(1:n-1,1);% Rotate x to change from 1 based indexing to 0 based
   g = ifft(y);
   f(1,1)=g(1,1);
   k = floor(n/2);
   for j=1:k-1
     f(2*j,1) = g(j+1,1) + g(n+1-j);
     f(2*j+1,1) = (g(j+1,1) - g(n+1-j))/i;
   f(n,1)=g(k+1,1);
   end
end

% Examples
>> dft([1;2;2;1])'
ans =
    1.5000   -0.5000   -0.5000         0
>> (trigBasis(2)\[1;2;2;1])'
ans =
    1.5000   -0.5000   -0.5000         0

>> dft([1;4;2;8;5;7])'
ans =
    4.5000    0.6667   -2.3094         0         0    1.8333
>> (trigBasis(3)\[1;4;2;8;5;7])'
ans =
    4.5000    0.6667   -2.3094   -0.0000   -0.0000    1.8333


% Converts column vector in frequency domain to vector in time domain.
%    using the real Fourier components discussed in the text
% Let X = < x[1] ... x[n] >
% Let F = idft(X)
% Then F[i] = X[1] + X[2] cos(pi i/N) + X[3] sin(pi i/N) +
%       ... X[N-2] cos(pi (N-1)/N) +X[N-1] sin(pi i (N-1)/N)) + X[N] cos(pi i).

% idft(x) is equal to trigBasis(N/2)*x but computes faster, since it uses
% the FFT.

function f = idft(x)
   n = size(x);
   n = n(1);
   k = floor(n/2);
   y(1,1)=x(1,1);
   for j=1:k-1
     y(j+1,1) = (x(2*j,1) + i * x(2*j+1,1))/2;
     y(n+1-j,1) = (x(2*j,1) - i * x(2*j+1,1))/2;
```

```
   end;
   y(k+1,1) = x(n,1);
   g = fft(y);
   f(n,1) = g(1,1);
   f(1:n-1,1) = g(2:n,1); % Rotate g to change from 0 based indexing to 1 based
end

% Examples

>> idft([1;2;2;1])'
ans =
     2     0    -2     4
>> (trigBasis(2)*[1;2;2;1])'
ans =
    2.0000    0.0000   -2.0000    4.0000

>> idft([1;4;2;8;5;7])'
ans =
   -1.9378   -0.5981   -2.0000    4.5981  -14.0622   20.0000

>> (trigBasis(3)*[1;4;2;8;5;7])'
ans =
   -1.9378   -0.5981   -2.0000    4.5981  -14.0622   20.0000

>> (trigBasis(3)*[1;4;2;8;5;7])'
ans =
   -1.9378   -0.5981   -2.0000    4.5981  -14.0622   20.0000
>> idft(dft([1;4;2;8;5;7]))'
ans =
    1.0000    4.0000    2.0000    8.0000    5.0000    7.0000
>> dft(idft([1;4;2;8;5;7]))'
ans =
    1.0000    4.0000    2.0000    8.0000    5.0000    7.0000
```

Exercises

Exercise 7.1

Let $\mathcal{C}$ be the coordinate system with origin $\mathbf{o}$, unit length d and unit coordinate arrow $\vec{x}$ and $\vec{y}$, and let $\mathcal{B}$ be the coordinate system with origin $\mathbf{p}$, unit length e and unit coordinate arrows $\vec{i}$ and $\vec{j}$.

Suppose that $\text{Coords}(\mathbf{p}, \mathcal{C}) = \langle 2, 3\rangle$, $\text{Coords}(e, \mathcal{C}) = 5$, $\text{Coords}(\vec{i}, \mathcal{C}) = \langle 4, 3\rangle$, and $\text{Coords}(\vec{j}, \mathcal{C}) = \langle -3, 4\rangle$.

A. Let $\mathbf{q}$ be the point with coordinates $\langle 1, 2\rangle$ in $\mathcal{B}$. What are the coordinates of $\mathbf{q}$ in $\mathcal{C}$?

B. Let $\mathbf{r}$ be the point with coordinates $\langle 1, 2\rangle$ in $\mathcal{C}$. What are the coordinates of $\mathbf{r}$ in $\mathcal{B}$?

Note: You should be able to solve (A) by hand. For (B), try to solve it by hand; if you get stuck, use MATLAB.

Exercise 7.2

Consider the 8×8 ill-conditioned matrix

```
1.001  1.002  1.003  1.004  1.005  1.006  1.007  1.009
1.002  1.003  1.004  1.005  1.006  1.007  1.008  1.010
1.003  1.004  1.005  1.006  1.007  1.008  1.010  1.011
1.004  1.005  1.006  1.007  1.008  1.010  1.011  1.012
1.005  1.006  1.007  1.008  1.010  1.011  1.012  1.013
1.006  1.007  1.008  1.010  1.011  1.012  1.013  1.014
1.007  1.008  1.010  1.011  1.012  1.013  1.014  1.015
1.008  1.010  1.011  1.012  1.013  1.014  1.015  1.016
```

discussed in section 5.5, page 115.

a. What is the condition number for this matrix? (Note: copying this from the 8×8 matrix shown above is error-prone; the matrix is not quite as regular as it appears at first glance. Copy the MATLAB code used to create it on p. 115.)

b. In the example given on page 115 let x be the second vector of constant terms and let $\tilde{x}$ be the first vector. Then the ratio of relative error in the answer to relative error in the constant terms is about 84,000, which is large but much less than the condition number. Construct an example where this ratio is close to the condition number.

Exercise 7.3

In this exercise, you will experiment with using singular value decomposition for image compression.

Step 1: Get hold of a gray scale image to play with. The course web site provided a 601 x 512 pixel grey-scale photograph of Abe Lincoln in lincoln.png to experiment with, but get another picture that you like.

Step 2: Load the image into an array $m \times n$ "Image", using the supplied function getimage.m.

```
Image = getimage('lincoln.png');
```

(This function is courtesy of Pascal Getreuer, in http://www.math.ucla.edu/ getreuer/matlabimaging.html)

Step 3: Carry out SVD decomposition on the image:

```
[L,S,R] = svd(Image);
R=R';
```

Step 4: For various small values of k, construct the k-th order approximation of Image, as described in the text:

> Let $S1$ be the $k \times k$ matrix with the first k singular values in S.
> Let $L1$ be the $m \times k$ matrix with the first k columns of L.
> Let $R1$ be the $k \times n$ matrix with the first k rows of R.
> Let $Image1 = L1 \cdot S1 \cdot R1$

Step 5: Print out the image, using the MATLAB function 'imwrite'. Pascal Getreuer recommends that images should be output in .png format.

```
imwrite(Image1,'<filename>')
```

Step 6: Pick a couple of characteristics of the image, and find the smallest values of k for which these characteristics are recognizable in the reconstructed image. For instance, for Abe Lincoln, you might choose to find the smallest values for which the image is recognizably a seated person, and the smallest value for which it is recognizably Lincoln.

You should submit the images you have found in step 6, together with a statement of what features you were looking for.

If you want to be ambitious, use a color image instead. The function "getimage" will return an $m \times n$ array, one layer for each primary color. Do SVD decompositions on each of the layers separately, and proceed as above.

If you want to be really ambitious, do this with several images of different visual characteristics — high contrast vs. low contrast, simple vs. complex, gray scale vs. line drawing — and try to get a feeling for when this works well, when badly, etc.

Problems

Problem 7.1

Let A be an $m \times n$ matrix, and let $A = L \cdot S \cdot R$ be the singular value decomposition of A. The *Moore-Penrose pseudoinverse* of A is the $n \times m$ matrix computed as follows: Let S' be the $n \times m$ diagonal matrix where each non-zero singular value σ in S is replaced by $1/\sigma$ and every zero singular value is left unchanged. Then the pseudoinverse A' is equal to $R^T \cdot S' \cdot L^T$.

For example, let

$$A = \begin{bmatrix} 13/9 & 11/9 & 13/9 & 11/9 \\ -23/18 & -25/18 & -23/18 & -25/18 \\ 5/9 & 7/9 & 5/9 & 7/9 \end{bmatrix}$$

Then the SVD of A is $A = L \cdot S \cdot R$ where

$$L = \begin{bmatrix} 2/3 & 2/3 & 1/3 \\ -2/3 & 1/3 & 2/3 \\ 1/3 & -2/3 & 2/3 \end{bmatrix} \qquad S = \begin{bmatrix} 4 & 0 & 0 & 0 \\ 0 & 1/3 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \qquad R = \begin{bmatrix} 1/2 & 1/2 & 1/2 & 1/2 \\ 1/2 & -1/2 & 1/2 & -1/2 \\ 1/2 & 1/2 & -1/2 & -1/2 \\ 1/2 & -1/2 & -1/2 & 1/2 \end{bmatrix}$$

Then

$$S' = \begin{bmatrix} 1/4 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

So

$$A' = R^T \cdot S' \cdot L^T = \begin{bmatrix} 13/12 & 5/12 & -23/24 \\ -11/12 & -7/12 & 25/24 \\ 13/12 & 5/12 & -23/24 \\ -11/12 & -7/12 & 25/24 \end{bmatrix}$$

Prove that, for *any* matrix A (*not* just the particular example above) if A' is the pseudoinverse then the following properties hold: (Hint: Keep in mind that L and R are orthogonal matrices, so $L^T = L^{-1}$ and $R^T = R^{-1}$.)

1. $A \cdot A' \cdot A = A$
2. $A' \cdot A \cdot A' = A'$
3. If A is a non-singular square matrix, then $A' = A^{-1}$.
4. $A \cdot A'$ and $A' \cdot A$ are both symmetric matrices. That is, if $B = A \cdot A'$ and $C = A' \cdot A$ then $B^T = B$ and $C^T = C$.

The converse is also true: For any matrix A, the only matrix that satisfies properties 1, 2, and 4 is the Moore-Penrose pseudoinverse of A. However, that is not easy to prove.

Problem 7.2

In section 6.4.7 we stated that, if A is a square matrix and Γ is the linear transformation corresponding to A, then, for an region R, $\text{Volume}(\Gamma(R)) = |\det(A)| \cdot \text{Volume}(R)$. Using this, show that, for any square matrix A, $|\det(A)|$ is equal to the product of the singular values of A.

Problem 7.3

A transformation Γ is a *projection* if, for all vectors $\vec{v}$, $\Gamma(\Gamma(\vec{v})) = \Gamma(\vec{v})$. (This is related to the geometric notion of projection, but a little different). Characterize a projection in terms of its singular values and of the relation between the right and left singular vectors.

Problem 7.4

Prove the following: If the right singular vectors of matrix A are all eigenvectors of A, then A is a symmetric matrix.

Problem 7.5

Any set $\mathcal{B}$ of n linearly independent n-dimensional vectors forms a basis for $\mathbb{R}^n$ and therefore any n-dimensional vector can be written as a linear sum over $\mathcal{B}$. Applying this to the 3-dimensional vector space of colors, that would seem to suggest that, if you take as your pallette three somewhat different shades of red, you can mix them to form any desired color, such as blue. That seems implausible. Resolve this apparent paradox.

Programming Assignments

Assignment 7.1

A *low-pass filter* is a signal processor that removes, or lessens, the high-frequency Fourier components of a signal while leaving the low-frequency components unchanged. A *high-pass filter* does the reverse.

Write two functions `LowPass(S,F)` and `HighPass(S,P)`. The input parameter S is a time signal over time interval [1,2N]. P is the cut-off period in one direction or the other. (The frequency is the reciprocal of the period.) The algorithms should proceeds as follows:

- Let T be the discrete Fourier transform of S.
- For the low-pass filter, set $T[k] \leftarrow 0$ for all $k > N/P$. For the high-pass filter, set $T[k] \leftarrow 0$ for all $k \leq N/P$.
- Return the inverse transform of the modified value of T.

Test your program on the square wave $S[i] = 1$ for $i = 1 \ldots 32$,$S[i] = -1$ for $i = 33 \ldots 60$. Plot the original signal, the Fourier coefficients, and the results of low-pass and high-pass filters for various values of N.

Part II

Probability

Chapter 8

Probability

Most of mathematics deals with statements that are known with certainty, or as least as much certainty as can be attained by fallible human beings. The statement "2+2=4" is the archetype of a statement that is known to be true. In a similar way, the objective in many types of computer software is to be entirely reliable, or at least as reliable as a machine that is built of silicon and is running a commercial operating system can be. We don't want compilers, or payroll data bases, or control systems for nuclear reactors, to give more or less correct answers most of the time; we want them to always work correctly; and to a substantial degree, this is often indeed an attainable goal.

But the reality of life is that we cannot work exclusively with information that is known with certainty. Often we must choose our actions as best we can on the basis of information that is partial and uncertain. Likewise, programs such as search engines, recommender systems, automatic translators and the like, whose results are not reliably correct, occupy an increasingly large and important segment of the world of software.[1] Therefore the mathematical theory of dealing with uncertain information has become increasingly important in many computer science applications. *Probability theory* is the fundamental theory of manipulating uncertainty.

8.1 The interpretations of probability theory

Probability theory has to do with assigning numbers, called *probabilities,* to entities of a certain kind, called *events*. For the remainder of this book, we will use the notation "$P(E)$" to mean the probability of event E.

Unfortunately, there are multiple, conflicting interpretations of probability theory, each with a different idea about what kind of entity an "event" is, and therefore a different idea of what probability theory is, fundamentally, *about*. (See Fine 1973 for a survey.) In this book we will look at two interpretations:

- The *sample space* or *frequentist* interpretation. In this interpretation, there is a fixed universe of entities Ω, called a sample space, and an event is a subset of the sample space. The probability of event E is the fraction of Ω that is in E.
- The *likelihood* or *subjectivist* interpretation. In this interpretation, an event E is a sentence or

[1] Even with programs where we expect and can get reliably correct answers, there may be other aspects where a probabilistic analysis is useful. For example, a database may introduce a query optimization that with high probability speeds up the computation of the answer.

a proposition. $P(E)$ is a judgement of how likely it is that E is true, as judged by a reasoner with some particular background knowledge.

We will first discuss the sample space interpretation, which is conceptually the simpler of the two theories. We will then turn to the likelihood interpretation, which is closer to the way that probability theory is used in the kinds of applications we will discuss. As we will see, though, the way that probability theory is used in applications does not fit perfectly with the likelihood interpretation either. There is, perhaps, yet another interpretation, the "application" interpretation implicit here; if so, no one has yet formulated what it is, very clearly.

8.2 Finite sample spaces

In the sample space interpretation of probability theory, all discussions of probabilities are carried out relative to a *probability space*. Probability spaces can be either finite or infinite; both cases are important and there are significant differences between them. We will deal with the infinite case in chapter 9. In this chapter, we will deal exclusively with finite spaces.

A finite probability space consists of two parts: a finite set Ω called the *sample space* and a real-valued function $P(x)$ over Ω called the *probability function* or *distribution*. The probability function has two properties:

F.1 For all $x \in \Omega$, $0 \leq P(x) \leq 1$.

F.2 $\sum_{x \in \Omega} P(x) = 1$.

An event is a subset of Ω. For any event E, the probability of E is the sum of the probabilities of its elements: $P(E) = \sum_{x \in E} P(x)$.

A set containing a single element of Ω is an *elementary event.*

A probability function that satisfies condition (2) above is said to be *normalized*. It is often convenient to deal with a more general class of weight functions $w(x)$ that satisfy the following weaker conditions:

W.1 For all $x \in \Omega$, $w(x) \geq 0$.

W.2 For some $x \in \Omega$, $w(x) > 0$.

We define the weight of any event E as the sum of the weights of the elements of E: $w(E) = \sum_{x \in E} w(x)$.

Clearly, if $P(x)$ is a probability function satisfying F.1 and F.2, then the weight function $w(x) = P(x)$ satisfies W.1 and W.2. Conversely, if weight function $w(x)$ satisfies W.1 and W.2, then we can *normalize* it by defining the associated probability function $P(x) = w(x)/w(\Omega)$. It is immediate that $P(x)$ so defined satisfies F.1 and F.2 and that for any event E, $P(E) = w(E)/w(\Omega)$.

The following examples are standard starting points for discussions of probability:

Example 8.1: You flip a fair coin. The sample space $\Omega =\{$ H, T $\}$. The probability function is $P(H) = 1/2$; $P(T) = 1/2$. The weight function $w(H) = w(T) = 1$ gives the same probability function. There are only 4 events in this sample space: $P(\emptyset) = 0$; $P(\{\text{H}\}) = 1/2$; $P(\{\text{T}\}) = 1/2$; $P(\Omega) = 1$. This probability function is called the *uniform* or *equiprobable* distribution, because all the elements of Ω have the same probability.

Example 8.2: You flip a weighted coin that comes up heads 3/4 of the time. The sample space $\Omega =\{$ H, T $\}$ The probability function is $P(\text{H}) = 3/4; P(\text{T}) = 1/4$.

Example 8.3: You roll a fair die. The sample space $\Omega = \{1, 2, 3, 4, 5, 6\}$. The probability function is the equiprobable distribution $P(x) = 1/6$ for each $x \in \Omega$. There are $64 = 2^6$ possible events here. For example:

- To compute the probability of rolling an even number, we use the event $E = \{2, 4, 6\}$, and computer $P(E) = P(2) + P(4) + P(6) = (1/6) + (1/6) + (1/6) = 3/6$.
- To compute the probability of rolling at least a 3, we use the event $E = \{3, 4, 5, 6\}$, and computer $P(E) = P(3) + P(4) + P(5) + P(6) = (1/6) + (1/6) + (1/6) + (1/6) = 4/6$.

When the probability is uniformly distributed, as in this example, we can equally well use the weight function $w(x) = 1$ for each $x \in \Omega$. Then for any event E, $w(E) = \#E$, the number of elements in E, so $P(E) = \#E/\#\Omega$.

Example 8.4: You flip a fair coin three times. The sample space here is the set of all eight possible outcomes:

$$\Omega = \{ \text{HHH, HHT, HTH, HTT, THH, THT, TTH, TTT} \}$$

The probability function is the uniform distribution, so, as remarked above, for any event E , $P(E) = \#E/\#\Omega$. For instance, if we want to know the probability of getting at least two heads, then $E=$ { HHT, HTH, THH } so $P(E) = \#E/\#\Omega = 3/8$.

8.3 Basic combinatorial formulas

Many probabilistic problems, such as computing the probability of getting a full house (3 of one number, two of another) in a five-card poker hand, require the use of combinatorial reasoning. On the whole combinatorics plays a smaller role in computer science applications of probability than in other kinds of applications; nonetheless, there are some basic formulas that everyone who is dealing with probability should know.

Exponential: The number of sequences of k items out of a set S of size n, allowing repetition, is n^k. For example, let $S = \{a, b\}$, $n = |S| = 2$, $k = 3$. Then the set of choices $C = \{aaa, aab, aba, abb, baa, bab, bba, bbb\}$ so $|C| = 8 = 2^3$. The argument is that each of the choices can be made in n ways independently of all the others; hence the total number of combinations is $n \cdot n \cdot \ldots \cdot n$ (k times) $= n^k$.

Permutations of n items: The number of sequences of all the elements, without repetition, in a set S of size n elements is called "n factorial" denoted $n!$, and computed as $n \cdot n - 1 \cdot \ldots \cdot 2 \cdot 1$. For instance, if $S = \{a, b, c, d\}$ and $|S| = n = 4$, then the set of permutations is

abcd	*abdc*	*acbd*	*acdb*	*adbc*	*adcb*
bacd	*badc*	*bcad*	*bcda*	*bdac*	*bdca*
cabd	*cadb*	*cbad*	*cbda*	*cdab*	*cdba*
dabc	*dacb*	*dbac*	*dbca*	*dcab*	*dcba*

and the number of permutations is $24 = 4! = 4 \cdot 3 \cdot 2 \cdot 1$.

The argument is that the first item can be chosen to be any of the n items in S. Having chosen the first, the second item can be chosen to be any of the remaining $n - 1$. Having chosen the first

two, the third item can be chosen to be any of the remaining $n-2$; and so on. The total number of combinations is therefore $n \cdot (n-1) \cdot (n-2) \cdot \ldots \cdot 2 \cdot 1 = n!$.

The MATLAB function `factorial(n)` computes $n!$.

Permutations of k items out of n: The number of sequences of k items chosen from a a set S of n items, with no repetitions, is known as the *permutations* of k out of n; it is sometimes notated $\mathrm{P}(n,k)$. It is computed as $n \cdot (n-1) \cdot (n-2) \cdot \ldots \cdot n-(k-1) = n!/(n-k)!$. The argument is that the first item can be chosen in n ways, the second item in $n-1$ ways ... the k item in $n-(k-1)$ ways. Note that the formula $P(n,k) = n!/(n-k)!$ works for the special case $k = n$ as well, if we posit that $0! = 1$; for this and other similar reason, it is standard to define $0! = 1$.

For example, let $S = \{a,b,c,d\}$ so $n = |S| = 4$, and let $k = 2$. Then the collection of sequences of 2 items is equal to $\{ab, ac, ad, ba, bc, bd, ca, cb, cd, da, db, cd\}$. The size of this set is $P(4,2) = 4!/2! = 4 \cdot 3 = 12$.

Combinations of k items out of n: The number of subsets of size k out of a set of size n is known as the *combinations of k in n*; it is often notated $C(n,k)$ or

$$C\begin{pmatrix} n \\ k \end{pmatrix} \qquad \text{or} \qquad \begin{pmatrix} n \\ k \end{pmatrix}$$

It is computed as $n!/k!(n-k)!$. The argument is as follows: Consider the list of permutations of k out of n discussed above. Each subset of size k appears in that list in each of the permutations of its elements; it therefore appears $k!$ times. Since the list of permutations has $n!/(n-k)!$ elements, the total number of subsets must be $(n!/(n-k)!)/k! = n!/(n-k)!k!$.

For example, let $S = \{a,b,c,d\}$ so $n = |S| = 4$, and let $k = 2$. Then the collection of subsets of size 2 is $\{a,b\}, \{a,c\}, \{a,d\}, \{b,c\}, \{b,d\}, \{c,d\}$. The number of such subsets is $4!/(2!\cdot 2!) = (4\cdot 3)/(2\cdot 1) = 6$.

The numbers $C(n,k)$ are also known as the *binomial coefficients*, because $C(n,k)$ is the coefficient of the term $x^k y^{n-k}$ in the expansion of $(x+y)^k$. These are also the numbers in Pascal's triangle; they satisfy the double recurrence $C(n,k) = C(n-1,k) + C(n-1,k-1)$. These numbers will figure prominently in our discussion of the binomial distribution (section 9.6.2)

The MATLAB function `nchoosek(n,k)` computes $C(n,k)$.

Partition into sets. Let $n = k_1 + k_2 + \ldots + k_m$. The number of ways of dividing a set S of size n into disjoint subsets $S_1 \ldots S_m$ where $|S_1| = k_1, |S_2| = k_2 \ldots |S_m| = k_m$ is often denoted $C(n : k_1 \ldots k_m)$ or as

$$\begin{pmatrix} & n & \\ k_1 & \ldots & k_m \end{pmatrix}$$

It is computed as $n!/(k_1! \cdot k_2! \cdot \ldots \cdot k_m!)$. The argument is as follows. First choose subset S_1 of size k_1 out of the whole set S; there are $C(n,k) = n!/k_1!(n-k_1)!$ possible choices. Now there are $n-k_1$ elements remaining, so the number of ways of choosing a set S_2 of size k_2 out of those is $C(n-k_1, k_2)$. Continuing on in this way, when we come to choose S_p there are $n - k_1 - k_2 - \ldots - k_{p-1}$ elements remaining, so the number of ways of choosing S_p is $C(n - k_1 - k_2 - \ldots - k_{p-1}, k_p)$. Multiplying all these together we get

$$C(n,k_1) \cdot C(n-k_1,k_2) \cdot C(n-k_1-k_2,k_3) \ldots =$$
$$\frac{n!}{k_1! \cdot (n-k_1)!} \cdot \frac{(n-k_1)!}{k_1! \cdot (n-k_1-k_2)!} \cdot \frac{(n-k_1-k_2)!}{k_3! \cdot (n-k_1-k_2-k_3)!} \cdot \ldots =$$
$$\frac{n!}{k_1! \cdot k_2! \cdot \ldots \cdot k_m!}$$

For example, let $S = \{a,b,c,d\}$ so $n = |S| = 4$, and let $k_1 = 2$, $k_2 = 1$, $k_3 = 1$. Then the collection of partitions is

S_1	S_2	S_3
$\{a,b\}$	$\{c\}$	$\{d\}$
$\{a,c\}$	$\{b\}$	$\{d\}$
$\{a,d\}$	$\{b\}$	$\{c\}$
$\{b,c\}$	$\{a\}$	$\{d\}$
$\{b,d\}$	$\{a\}$	$\{c\}$
$\{c,d\}$	$\{a\}$	$\{b\}$

S_1	S_2	S_3
$\{a,b\}$	$\{d\}$	$\{c\}$
$\{a,c\}$	$\{d\}$	$\{b\}$
$\{a,d\}$	$\{c\}$	$\{b\}$
$\{b,c\}$	$\{d\}$	$\{a\}$
$\{b,d\}$	$\{c\}$	$\{a\}$
$\{c,d\}$	$\{b\}$	$\{a\}$

The number of partitions is $4!/(2! \cdot 1! \cdot 1!) = 12$.

Stirling's formula gives a useful approximation for $n!$:

$$n! \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$$

Taking the natural logarithm of both sides and keeping only the two largest terms gives $\ln(n!) \approx n \ln n - n$

For example, $10! = 3,628,800$; Stirling's formula gives 3,598,695.62, a relative error of 0.8%.

Approximation of central binomial. As we will discuss further in section 9.8.2, the central term of the combinatorial function $C(n, n/2)$ is approximately equal to $2^n \cdot \sqrt{2/\pi n}$. For example, C(20,10)=184,756; this approximation gives a value of 187,078.97, a relative error of 1.2%

Example 8.5: You deal a poker hand of five cards from a 52-card deck. Here the sample space Ω is the set of all five-card hands, and the probability function is the uniform distribution. A five-card hand is thus a combination of 5 items out of 52; the size of Ω, $\#\Omega = C(52,5) = 52!/(47! * 5!) = 2,598,960$.

If we want to know the probability that an unseen hand is a flush, then the event E is the set of all hands that are flushes. Since we are using the uniform distribution, $P(E) = \#E/\#\Omega$. To count the number of hands that are flushes, we reason that the flush may be in any of the four suits. To construct a flush in spades, for example, we must choose 5 cards out of the 13 spades; the number of ways of doing this is $C(13,5)$. The total number of flushes in any suit is therefore $\#E = 4 * C(13,5) = 4 * 13!/(8! * 5!) = 5148$. Therefore $P(E) = 5148/2,598,960 = 0.002$.

Example 8.6: You have an urn containing 4 red balls and 9 black balls. Three times you pick a ball out of the urn, note its color, and put it back in the urn. (This is called "sampling with replacement".)

To construct the sample space, we will give each ball a number; we will number the red balls 1-4 and we will number the black balls 5-13. The sample space Ω is then just all triples of balls where a triple can include a repetition:

$$\Omega = \{\langle 1,1,1\rangle,\ \langle 1,1,2\rangle, \ldots \langle 1,1,13\rangle,\ \langle 1,2,1\rangle, \ldots \langle 13,13,12\rangle,\ \langle 13,13,13\rangle\}$$

The probability function is again the uniform distribution. The event "Exactly one ball is red" is the subset of all triples containing one red ball: $E = \{\langle 1,5,5\rangle,\ \langle 1,5,6\rangle \ldots \langle 13,13,4\rangle$. The total number of drawing three balls is $13^3 = 2197$. To count the number of draws that have exactly one red ball, we reason that the red ball may be either the first, the second, or the third drawn. If we consider the draws in which the first ball is red and other two are black, then there are 4 ways to choose the first ball, and 9 ways to choose each of the other two black balls, for a total of 4*9*9 possibilities. Since there are three possible positions of the red ball, the total number of draws with 1 red ball, $\#E = 3 * 4 * 9 * 9 = 972$. Therefore $P(E) = 972/2197 = 0.442$.

Example 8.7: You have an urn containing 4 red balls and 9 black balls. You pick three balls out of the urn without putting them back. (This is called "sampling without replacement".)

We number the balls as in example 8.6. The sample space Ω is then just all triples of balls with no repetitions in the triples:

$$\Omega = \{\langle 1,2,3\rangle,\ \langle 1,2,4\rangle, \ldots \langle 1,2,13\rangle,\ \langle 1,3,2\rangle, \ldots \langle 13,12,10\rangle,\ \langle 13,12,11\rangle\}$$

An element of Ω is a permutation of 3 balls out of the 13, so $\#\Omega = P(13,3) = 13 * 12 * 11 = 1716$.

Let E be the event that a draw has exactly one red ball. The calculation to compute $\#E$ is the same as in example 8.6 except that, when you come to draw the second black ball, there are only 8 possible choices, not 9. Therefore, the total number of such draws $\#E = 3 * 4 * 9 * 8 = 864$ so $P(E) = \#E/\#\Omega = 0.503$.

The poker hand of example 8.5 is also an example of sampling without replacement; the deck corresponds to the urn and the cards correspond to the balls. (Each card has a different color.) If we were to deal one card at a time, replace it in the deck, shuffle, and deal again, then that would be sampling with replacement.

8.4 The axioms of probability theory

The theory presented in the previous section takes as its starting point the function $P(x)$ where $x \in \Omega$. However, this approach works only in the case of finite sample spaces. A more general approach to axiomatizing of probability theory is based on events, which are the common coin of all probabilistic theories. In this approach, there are four axioms of probability theory:

P.1 For any event E, $0 \leq P(E) \leq 1$.

P.2 For any events E and F, if $E \cap F = \emptyset$ then $P(E \cup F) = P(E) + P(F)$.

P.3 $P(\emptyset) = 0$.

P.4 $P(\Omega) = 1$.

It is easy to prove that these four axioms are consequences of axioms F.1 and F.2, together with the definition $P(E) = \sum_{x \in E} P(x)$.

It is also possible to prove that P.1—P.4 are *all* the axioms of probability theory that you need, in the following sense: Suppose you have a collection of facts about probabilities of different events and their combinations. For example suppose you are told the following facts:

$P(A) = 0.2$.
$P(B) = 0.7$.
$P(A \cap B) = 0.1$.
$P(C \cup B) = 0.9$.
$P(C \setminus (A \cap B)) = 0.4$.

If this collection of facts is consistent with the axioms P.1—P.4 then you can construct a sample space and a probability function and assign each event to a subset of the sample space, in a way that makes all these statements true. In the terminology of axiomatic theory, this set of axioms is *complete* for sample space models.

One model of the above system of constraints would be:

$\Omega = \{v, w, x, y, z\}$.
$A = \{v, w\}$.
$B = \{v, x, y\}$.
$C = \{v, y, z\}$.

$P(v) = 0.1$.
$P(w) = 0.1$.
$P(x) = 0.4$.
$P(y) = 0.2$.
$P(z) = 0.2$.

Then
$P(A) = P(\{v, w\}) = 0.2$
$P(B) = P(\{v, x, y\}) = 0.7$
$P(A \cap B) = P(\{v\}) = 0.1$
$P(C \cup B) = P(\{v, x, y.z\}) = 0.9$
$P(C \setminus (A \cap B)) = P(\{y.z\}) = 0.4$

The following result is simple but important; it can easily be proved either from axioms P.1—P.4 or from axioms F.1 and F.2:

Definition 8.1. *Two events E and F are* mutually exclusive *if $E \cap F = \emptyset$.*

A collection of events $\{E_1 \dots E_k\}$ forms a frame of discernment *if every element x is in exactly one E_i. Equivalently,*

- *for $i \neq j$, $E_i \cap E_j$ are mutually exclusive.*
- $E_1 \cup E_2 \cup \dots \cup E_k = \Omega$.

Theorem 8.1. *Let $\mathcal{E} = \{E_1 \dots E_k\}$ be a collection of events. If every pair of events $E_i, E_j, i \neq j$ in $\mathcal{E}$ are mutually exclusive then $P(E_1 \cup \dots \cup E_k) = P(E_1) + \dots + P(E_k)$. In particular, if $\{E_1 \dots E_k\}$ forms a frame of discernment then $P(E_1) + P(E_2) + \dots + P(E_k) = P(\Omega) = 1$.*

8.5 Conditional probability

Let E and F be events and assume that $P(F) > 0$. The *conditional probability of E given F,* denoted $P(E|F)$ is the fraction of F that is also E. In other words, we shrink the sample space from Ω to F while keeping the weight function unchanged, and now consider the probability of E within this restricted space. Probabilities with no conditional, such as we have been considering previously, are called *absolute* probabilities.

Once we have restricted the space to be F, the part of E that is significant is just $E \cap F$. Therefore, the probability of E within the sample space F is $P(E|F) = w(E \cap F)/w(F)$. Now if we divide both numerator and denominator by $w(\Omega)$ we have

$$P(E|F) = \frac{w(E \cap F)/w(\Omega)}{w(F)/w(\Omega)} = \frac{P(E \cap F)}{P(F)}$$

This is the *conditional probability formula.* Multiplying through gives us the *conjunction formula*: $P(E \cap F) = P(F) \cdot P(E|F)$.

Example 8.3, revisited: Let Ω be the sample space of all eight outcomes of flipping a coin three times, and let $P(x) = 1/8$ for each outcome x. Let F be the event of getting exactly two heads and let

E be the event that the first flip is heads. Thus E= { HHH, HHT, HTH, HTT }; F = { HHT, HTH, THH }; and $E \cap F$ = { HHT, HTH }. Therefore $P(E|F) = P(E \cap F)/P(F) = (2/8)/(3/8) = 2/3$, and $P(F|E) = P(E \cap F)/P(E) = (2/8)/(4/8) = 1/2$.

Since conditioning probabilities on event G is simply a change in the sample space, it follows that any formula that holds generally for absolute probabilities also holds if some event G is added as a condition across the board. For instance we can add G as a condition to each of the axioms P.1-P.4; the results are the following axioms C.1-C.4:

C.1 For any event E , $0 \leq P(E|G) \leq 1$.

C.2 For any events E and F, if $E \cap F \cap G = \emptyset$ then $P(E \cup F|G) = P(E|G) + P(F|G)$.

C.3 If $E \cap G = \emptyset$ then $P(E|G) = 0$.

C.4 $P(G|G) = 1$.

We can also add G as a condition in the conjunction formula:

$$P(E \cap F|G) = \frac{P(E \cap F \cap G)}{P(G)} = \frac{P(E \cap F \cap G)}{P(F \cap G)} \cdot \frac{P(F \cap G)}{P(G)} = P(E|F \cap G) \cdot P(F|G)$$

Note that this is the same as the formula $P(E \cap F) = P(E|F)P(F)$ with the additional condition G added across the board. Indeed, if you have any theorem of probability theory involving a combination of absolute and conditional probabilities, it remains true if you add G as an additional condition to each probability term.

The conjunction formula can be extended to cover the conjunction of any number of events. For three events E, F, G we have

$$P(E \cap F \cap G) = P(E|F \cap G)P(F \cap G) = P(E|F \cap G) \cdot P(F|G) \cdot P(G)$$

For k events, we have

$$P(E_1 \cup E_2 \cup \ldots \cup E_k) = P(E_1|E2 \cup \ldots E_k) \cdot P(E_2|E3 \cup \ldots E_k) \cdot \ldots \cdot P(E_{k-1}|E_k) \cdot P(E_k)$$

8.6 The likelihood interpretation

The sample space model of probability is clear and coherent and is well suited to many kinds of problems. However, many of the applications where we need to reason with uncertain information do not fit this model at all well. Consider the following:

1. Given the text of an email message, what is the likelihood that it is spam?
2. Given a search query and the text of a web page, what is the likelihood that the page is relevant to the query?
3. Given the form of an image, what is the likelihood that it shows an airplane?
4. Given a patient's personal history and medical record, what is the likelihood that she has diabetes?

What happens if we try to analyze these kinds of examples in terms of a sample space? Consider problem 4, of a medical diagnosis. The sample space Ω is presumably the set of all people; or, better, the set of all pairs of a person and a day, such as $\langle Marilyn\ O'Reilly, 4/7/2008\rangle$. We want to determine $P(E|F)$ where E is diabetes and F is the medical record. More precisely, in the sample space model, the event E is the set of $\langle P, D\rangle$ such that P had diabetes on day D; and the event F is the set of $\langle P, D\rangle$ of people who on day D had the specified medical record. The problem is that, if the medical record is detailed enough, with, say, a long history of precise test results, and a large set of answers to personally intrusive questions, then, in this history of the medical profession, only one person on one day has had exactly that medical record; namely Marilyn O'Reilly herself, on April 7, 2008. So F is the singleton set $\{\langle Marilyn\ O'Reilly, 4/7/2008\rangle\}$ and $E \cap F$ is either equal to F, if Marilyn had diabetes on that date, or equal to the empty set, if she did not. So if Marilyn had diabetes on that date, then $E = F$ and $P(E|F) = 1$; if she didn't, then $E = \emptyset$ and $P(E|F) = 0$. We don't know which, until we determine whether she had diabetes. Clearly, this is not getting us where we want to go. The other examples above run into similar kinds of trouble. Indeed, many standard probability textbooks assert specifically that it is meaningless to speak of "the probability that Marilyn O'Reilly has diabetes", or even, strictly speaking, "the probability that the next time I flip a coin it will come up heads"; probabilities, they say, are only meaningful as applied to general categories.

In order to apply probability to examples like the diagnosis problem, we use the likelihood interpretation of probability theory. In this theory, an *event* is a proposition like "Marilyn O'Reilly has diabetes," "Marilyn O'Reilly has a blood glucose level of 150 mg/dL", "Marilyn O'Reilly does vigorous exercise at the gym three times a week", and so on. There is an implicit (in practice, usually rather rich) background body of knowledge. For example, in the diagnosis domain, this background knowledge might include general information about frequency of different conditions in the population and the general relation between diagnoses and medical test results and measurements, but no facts about individual patients. Then $P(E)$ is the likelihood that E is true given only the background knowledge. $P(E|F)$ is the likelihood that E is true if one learns F in addition to the background knowledge. In the diabetes example, E is the proposition "Marilyn O'Reilly has diabetes on 4/7/2008" and F is the conjunction of all the facts in her medical record. In the spam example E is the proposition, "Message 12472 is spam" and F is the proposition "The text of message 12472 is $\langle$ whatever it is $\rangle$".

So now it is a meaningful question to ask, "What is $P(E|F)$?"; it means "How likely is it that Marilyn has diabetes, if we are told her medical record in addition to our background knowledge?" This is certainly the right question to be asking, so we have at least made some progress over the sample space theory in which it is a meaningless question. However the analysis does not, in itself, provide any guidance whatever about how to calculate the answer.

It is not at all obvious that "likelihood" in this sense is a coherent enough notion to allow mathematical treatment. However, the theory of subjective probability posits that a mathematical analysis is indeed possible, and that, in fact, the measurement of likelihood observes the axioms of probability S.1–S.5 below. A number of different kinds of arguments have been advanced to justify the use of these axioms; see (Fine 1973). For our purposes we will simply accept the probabilistic model of likelihood, because (a) it is clearly a reasonable model in the case where the likelihood judgment is based on a sample space; (b) it has been found to work well in practice.

In this view, a probabilistic event is a *sentence* within a *propositional language*. A propositional language consists of three parts:

- The two *truth constants* $\top$ (true) and $\bot$ (false).
- A set of *propositional atoms*. We will use boldface symbols such as $\mathbf{Q}$, $\mathbf{R}$ etc. for propositional atoms.

- The Boolean operators $E \wedge F$ (E and F), $E \vee F$ (E or F), $E \Rightarrow F$ (E implies F), $E \Leftrightarrow F$ (E if and only if F), and $\neg E$ (not E). These allow two simple sentences E and F to be combined into a compound sentence.

A *sentence* is a combination of propositional atoms and truth constants using the Boolean operators. The relations between sentences are defined in the *propositional calculus*, also called *Boolean logic*. We assume the readers are familiar with the propositional calculus

The subjective theory of probabilities posits that the probability function satisfies the following axioms S.1-S.6.

S.1 For any sentence E, $0 \leq P(E) \leq 1$.

S.2 If it is known that $\neg(E \wedge F)$ then $P(E \vee F) = P(E) + P(F)$.

S.3 $P(\top) = 1$.

S.4 $P(\bot) = 0$.

S.5 If it is known that $E \Leftrightarrow F$, then $P(E) = P(F)$.

In particular, both S.2 and S.5 hold in the case where the sentence in question is known because it is a logical truth. For example, it is a theorem of propositional logic that $(A \vee B) \Leftrightarrow \neg(\neg A \wedge \neg B)$; therefore, one can apply axiom S.5 and conclude that that $P(A \vee B) = P(\neg(\neg A \wedge \neg B))$.

As you can see, these are largely the same as axioms P.1—P.4 in the frequentist theory. There are two differences. First, the set operators $\cup$ and $\cap$ have been changed to the propositional operators $\vee$ and $\wedge$. Second, axiom S.5 has been added. This reflects the fact that set theory and propositional logic use different conventions about equality; in set theory, two sets that contain the same elements are equal, whereas in propositional logic two sentences that have the same truth conditions are considered unequal if they have different forms.

We define conditional probability in the same way as in the frequentist theory:
$P(E|F) \equiv P(E \wedge F)/P(F)$.

8.7 Relation between likelihood and sample space probability

The likelihood theory and the sample space theory are closely related; they end up in much the same place, though they approach it from different directions.

Suppose that you have a finite set $\mathcal{S} = \mathbf{P}_1 \ldots \mathbf{P}_k$ of propositional atoms in mind. Then you can define an *elementary event* to be the conjunction of either the positive or the negative of all the atoms; and you can define a sample space to be the set of all elementary events, with the associated probability.

For example, suppose the three propositional atoms are $\mathbf{P}, \mathbf{Q}, \mathbf{R}$. Then the associated sample space Ω is $\{E_1 \ldots E_8\}$ where

$E_1 = \mathbf{P} \wedge \mathbf{Q} \wedge \mathbf{R}$.
$E_2 = \mathbf{P} \wedge \mathbf{Q} \wedge \neg\mathbf{R}$.
$E_3 = \mathbf{P} \wedge \neg\mathbf{Q} \wedge \mathbf{R}$.
$E_4 = \mathbf{P} \wedge \neg\mathbf{Q} \wedge \neg\mathbf{R}$.

$E_5 = \neg\mathbf{P} \wedge \mathbf{Q} \wedge \mathbf{R}$.
$E_6 = \neg\mathbf{P} \wedge \mathbf{Q} \wedge \neg\mathbf{R}$.
$E_7 = \neg\mathbf{P} \wedge \neg\mathbf{Q} \wedge \mathbf{R}$.
$E_8 = \neg\mathbf{P} \wedge \neg\mathbf{Q} \wedge \neg\mathbf{R}$.

There are two important points about this. First, exactly one of these elementary events must be true. That is, it is a theorem of the propositional calculus that

$E_1 \vee E_2 \vee E_3 \vee E_4 \vee E_5 \vee E_6 \vee E_7 \vee E_8$; and
for each $i \neq j$, $\neg(E_1 \wedge E_j)$.

The analogue of theorem 8.1 can be proven from axioms S.1-S.5, so

$$P(E_1) + P(E_2) + P(E_3) + P(E_4) + P(E_5) + P(E_6) + P(E_7) + P(E_8) = 1.$$

Therefore these probabilities are a valid probability function over the sample space Ω. This probability function is known as the *joint probability distribution* over the set of propositional atoms $\mathbf{P}, \mathbf{Q}, \mathbf{R}$.

Second, each of these elementary events corresponds to one line in a truth table. If you know that some particular elementary event E_i is true, then that determines the truth or falsehood of any sentence F over these propositional atoms. For example if the sentence $E_3 = \mathbf{P} \wedge \neg\mathbf{Q} \wedge \mathbf{R}$ is true, then $\mathbf{P}$ is true, $\mathbf{Q}$ is false, and $\mathbf{R}$ is true, so $\mathbf{P} \wedge \mathbf{Q}$ is true, $\neg\mathbf{P} \vee \mathbf{Q}$ is false $\neg(\mathbf{P} \wedge \mathbf{R}) \vee \mathbf{Q}$ is false, and so on. Therefore, any sentence F is logically equivalent to the disjunction of some of the elementary events; namely, all the sentences E_i that would make F true. For example

$\mathbf{P} \wedge \mathbf{Q} \equiv E_1 \vee E_2$
$\neg\mathbf{P} \vee \mathbf{Q} \equiv E_1 \vee E_2 \vee E_5 \vee E_6 \vee E_7 \vee E_8$.
$\neg(\mathbf{P} \wedge \mathbf{R}) \vee \mathbf{Q} \equiv E_1 \vee E_2 \vee E_5 \vee E_6 \vee E_7$.

However, since the E_i's are mutually exclusive, it follows that the probability of any disjunction of E_i's is just the sum of their probabilities:

$$\begin{aligned}
&P(\mathbf{P} \wedge \mathbf{Q}) = P(E_1 \vee E_2) = P(E_1) + P(E_2) \\
&P(\neg\mathbf{P} \vee \mathbf{Q}) = P(E_1 \vee E_2 \vee E_5 \vee E_6 \vee E_7 \vee E_8) = \\
&\qquad P(E_1) + P(E_2) + P(E_5) + P(E_6) + P(E_7) + P(E_8) \\
&P(\neg(\mathbf{P} \wedge \mathbf{R}) \vee \mathbf{Q}) = P(E_1 \vee E_2 \vee E_5 \vee E_6 \vee E_7) = \\
&\qquad P(E_1) + P(E_2) + P(E_5) + P(E_6) + P(E_7).
\end{aligned}$$

So we can identify the sentence $\mathbf{P} \wedge \mathbf{Q}$ with the set $\{E_1, E_2\}$; we can identify the sentence $\neg\mathbf{P} \vee \mathbf{Q}$ with the set $\{E_1, E_2, E_5, E_6, E_7, E_8\}$; and so on.

Thus, for any finite subjective theory there is a finite sample space, and vice versa. However, the two views develop the theory in opposite directions. With finite sample spaces we start with the elements and combine them into sets to form events. With a finite propositional theory, we start with events and combine them with conjunction and negation to form elements. As we will see in chapter 9, in the more general setting which includes infinite sample spaces, the theory starts and ends with events; it never reaches elements.

8.8 Bayes' law

Bayes' Law is a simple but powerful rule that governs reversing the direction of conditional probabilities.

By the rule of conjunction $P(E \wedge F) = P(E) \cdot P(F|E)$. Also $P(E \wedge F) = P(F) \cdot P(E|F)$. So $P(F) \cdot P(E|F) = P(E) \cdot P(F|E)$. Dividing through by $P(F)$ we get

$$P(E|F) = \frac{P(E) \cdot P(F|E)}{P(F)}$$

That is Bayes' Law.

This is important in the cases where you want to know the number on the left, and you do know (or can guess) the numbers on the right. In many cases of that kind, you don't actually know $P(F)$ directly, Rather you know that E is one of a frame of discernment $\{E = E_1, E_2 \ldots E_k\}$ and you know $P(E_i)$ and $P(F|E_i)$ for each E_i. Then you can compute $P(F)$ as follows: Since $\{E_1 \ldots E_k\}$ is a frame of discernment it follows that

- for $i \neq j$, $F \wedge E_i$ and $F \wedge E_j$ are mutually exclusive;
- $F = (F \wedge E_1) \vee (F \wedge E_2) \vee \ldots \vee (F \wedge E_k)$.

Therefore $P(F) = P(F \wedge E_1) + \ldots + P(F \wedge E_k)$. So we can rewrite Bayes' law in the following form:

$$P(E_i|F) = \frac{P(E_i) \cdot P(F|E_i)}{P(E_1) \cdot P(F|E_1) + \ldots + P(E_k) \cdot P(F|E_k)}$$

For example: A patient sees a doctor for a regular checkup. The doctor decides that it would be a good idea to test the patient for disease D; this disease affects 1 in every 10,000 people. There is a test T for D that is 99% accurate; that is, if the patient has D then with 99% probability the test will come up positive; if the patient does not have D then with 99% probability the test will come up negative. Sadly the test comes up positive. What is the probability that the patient has D?

Answer: By Bayes' Law

$$P(D|T) = \frac{P(D) \cdot P(T|D)}{P(D) \cdot P(T|D) + P(\neg D) \cdot P(T|\neg D)}$$

We are given that $P(D) = 0.0001$, $P(T|D) = 0.99$, $P(T|\neg D) = 0.01$. Also $P(\neg D) = 1 - P(D) = 0.9999$. So $P(D|T) = (0.99 * 0.0001)/((0.99 * 0.0001) + (0.01 * 0.9999) = 0.0098$, slightly less than 1 in 100.

This seems surprising at first, but is actually reasonable. Suppose the doctor tests 10,000 people. One of them has D, and the test will come up positive. 9,999 don't have D; the test will come up positive for roughly 100 of those. So there will be 101 patients with positive results, only one of whom actually has the disease. In general, in this kind of reasoning, people tend to give too much weight to the accuracy of the test $P(T|D)$, and not nearly enough to the base rate $P(D)$.

Note, however, that this only applies if the people whom the doctor is testing are a random sample of the population. If the doctor has some particular reason for testing the patient — for instance, the patient is complaining of symptoms, or the patient is a member of some population who is at risk (age, ethnic group, etc.) — then this calculation does not apply, because there is additional information that must be taken into account. Then we face the problem of evidence combination, which we will discuss in section 8.9.1.

8.9 Independence

A critical component of probability theory is the observation that *most events have nothing whatever to do with one another.* Finding out whether it is raining in Poughkeepsie does not at all influence our estimate of the likelihood that the yen will gain against the dollar tomorrow. The usability of the theory of probability, and indeed the possibility of rational thought, rests on this disconnection. If we had to rethink the likelihood of everything each time we learned a new fact, then thinking would be pretty much impossible.

The mathematical notion here is *independence*:

Definition 8.2. *Event E is independent of F if learning F does not affect the estimate of the likelihood of E. That is, $P(E|F) = P(E)$.*

(It is noteworthy that the natural definition is in terms of the likelihood interpretation of probability. The concept of independence seems much more arbitrary when viewed in terms of the sample space interpretation.)

Note that the condition $P(E|F) = P(E)$ is equivalent to $P(E, F)/P(F) = P(E)$. This leads to two important consequences:

1. $P(E, F) = P(E) \cdot P(F)$. This is a simpler version of the general rule of conjunction. We emphasize that this *only* applies if E and F are independent.
2. $P(F|E) = P(E, F)/P(E) = P(F)$. Thus, if E is independent of F, then F is independent of E. So independence is a *symmetric* relation, which is not obvious from our original definition.

Notational note: We are using here a standard notation of probability theory in which E, F means $E \wedge F$, within a probability operator. Thus $P(E, F)$ means $P(E \wedge F)$; $P(E|F, G)$ means $P(E|F \wedge G)$, and so on.

Like other aspects of probability, independence can be conditionalized:

Definition 8.3. *Let E, F, G be events. Event E is* conditionally independent of F given G *if, after you have learned G, additionally learning F does not affect the likelihood of E. That is $P(E \mid F, G) = P(E \mid G)$.*

By the same argument as above, if E is conditionally independent of F given G, then the following two statements hold:

$P(F|E, G) = P(F|G)$; that is, F is conditionally independent of E given G.
$P(E, F|G) = P(E|G) \cdot P(F|G)$.

Independence also applies to larger collections of events:

Definition 8.4. *A collection of events $\{E_1 \dots E_k\}$ is independent if finding out the values of any subset does not affect the likelihood of the rest. That is, if S is a subset of the events and $E_i \notin S$, then $P(E_i|S) = P(E_i)$.*

If $\{E_1 \dots E_k\}$ is independent then $P(E_1 \dots E_k) = P(E_1) \cdot P(E_2) \cdot \dots \cdot P(E_k)$.

It is possible to have a collection of events in which every pair is independent but the collection as a whole is not independent. We will see an example where this is important in section 8.9.2.

Example 8.3, revisited: You flip a coin three times. Let H_1, H_2, H_3 be the events that the 1st, 2nd, and 3rd flips come up heads. Then these three are independent, so $P(H_1, H_2, H_3) = 1/8$, agreeing with our earlier calculation from the sample space.

Example 8.6: revisited: You have an urn with 4 red balls and 9 black balls, and you sample with replacement three times. Let R_1, R_2, R_3 be the events that the three samples are red. Then these three are independent, each time you are sampling from the same collection.

Example 8.7: revisited: You have an urn with 4 red balls and 9 black balls, and you sample without replacement three times. Let R_1, R_2, R_3 be the events that the three samples are red. Then these three events are *not* independent. Since 4 out of the 13 balls are red, and, before you start, all the balls are equally likely to be picked on the second draw, the absolute probability $P(R_2) = 4/13$. If R_1 is true, then when you pick the second ball, there are 12 balls in the urn of which 3 are red, so $P(R_2|R_1) = 3/12$. If R_1 is false, then when you pick the second ball, there are 12 balls in the urn of which 4 are red, so $P(R_2|\neg R_1) = 4/12$.

8.9.1 Independent evidence

Suppose that we want to determine the likelihood of some proposition X, and we have two pieces of evidence E and F. Both E and F are each quite good evidence for the truth of X. Specifically the absolute probability $P(X) = 1/3$, the conditional probabilities $P(X|E) = 0.8$ and $P(X|F) = 0.9$, so both E and F very much raise the likelihood of X. What can we say about the probability of $P(X|E, F)$?

The answer is that we can't say anything at all. $P(X|E, F)$ can have any value from 0 to 1 inclusive. The intuitive justification is that you can construct a model in which $E \cap F$ is only a very small fraction of E and of F, and so it is consistent with the constraints on $P(X|E)$ and $P(X|F)$ either that X covers $E \cap F$ or that X is disjoint from $E \cap F$.

For example, we can satisfy the constraints $P(X) = 1/3$, $P(X|E) = 0.8$, $P(X|F) = 0.9$, $P(X|E, F) = 0.01$ using the following probability space.

Ω = { a,b,c,d,e,f,g }.
E = { a,b,c,d }.
F = { a,b,e,f }.
X = { a,c,e }.
w(a)=1. w(b)=99. w(c)=799. w(d)=101. w(e)=899. w(f)=1. w(g)=3800.

This generalizes to any number of pieces of evidence. You can have evidence $E_1 \ldots E_k$ in which each fact individually is good evidence for X, and any pair of facts is strong evidence for X, and any three facts is very strong evidence for X ...and any collection of $k - 1$ facts is overwhelming evidence for X, and yet $P(X|E_1 \ldots E_k) = 0$. In fact we have the following theorem.

Theorem 8.2. *Let X and $E_1 \ldots E_k$ be variables ranging over events. Let $m = 2^k$. Let $S_1 \ldots S_m$ be the m subsets of $\{E_1 \ldots E_k\}$. Let $\langle c_1 \ldots c_m \rangle$ be any 2^k-tuple of numbers strictly between 0 and 1. Then the system of equations $\{P(X|S_1) = c_1, \ldots, P(X|S_m) = c_m\}$ is consistent. That is, there exists a sample space Ω, a probability function P and an assignment of X and of all the E_i to events in Ω that satisfies all these equations.*

The proof is left as a rather difficult exercise (problem 8.2).

Let us return to our problem. We have $P(X) = 1/3$, $P(X|E) = 0.8$, $P(X|F) = 0.9$, but we can't get any direct information about $P(X|E, F)$. What can we do?

This is a common — in fact, almost universal — situation in applied probabilistic reasoning: you have a situation involving a combination of many events, and you can't get direct information about the statistics of the entire combination. Standard operating procedure in this situation is that you use independence assumptions to split the large combination into smaller groups about which you do have information. In this case, we don't have information about the combination X, E, F, but we do have information about each of the pairs X, E and X, F, so we have to find a set of independence assumptions that will allow us to analyze X, E, F in terms of X, E and X, F.

In this particular case, the usual independence assumption is to posit that E and F are conditionally independent, both given X and given $\neg X$. (In section 13.6.1, we will present an argument justifying the choice of this particular independence assumption.) That is $P(E, F|X) = P(E|X) \cdot P(F|X)$ and $P(E, F|\neg X) = P(E|\neg X) \cdot P(F|\neg X)$

We now proceed as follows. By Bayes' law

$$P(X|E, F) = \frac{P(E, F|X) \cdot P(X)}{P(E, F)} \tag{8.1}$$

Likewise

$$P(\neg X|E, F) = \frac{P(E, F|\neg X) \cdot P(\neg X)}{P(E, F)} \tag{8.2}$$

Dividing equation 8.1 by equation 8.2 gives

$$\frac{P(X|E, F)}{P(\neg X|E, F)} = \frac{P(E, F|X) \cdot P(X)}{P(E, F| \neg X) \cdot P(\neg X)} \tag{8.3}$$

Applying the independence assumptions, we get

$$\frac{P(X|E, F)}{P(\neg X|E, F)} = \frac{P(E|X) \cdot P(F|X) \cdot P(X)}{P(E| \neg X) \cdot P(F| \neg X) \cdot P(\neg X)} \tag{8.4}$$

For any events A, B, let us define the odds on A as $\text{Odds}(A) = P(A)/P(\neg A)$, and the conditional odds on A given B, $\text{Odds}(A|B) = P(A|B)/P(\neg A|B)$. For example, if $P(A) = 3/4$ then $\text{Odds}(A) = (3/4)/(1/4) = 3$. (These are the "3 to 1 odds" used at the racetrack.) Note that $\text{Odds}(A) = P(A)/P(\neg A) = P(A)/(1 - P(A))$; solving for $P(A)$ we have $P(A) = \text{Odds}(A)/(1 + \text{Odds}(A))$. Likewise $\text{Odds}(A|B) = P(A|B)/(1 - P(A|B))$ and $P(A|B) = \text{Odds}(A|B)/(1 + \text{Odds}(A|B))$. Moreover, by Bayes' law

$$\text{Odds}(A|B) = \frac{P(A|B)}{P(\neg A|B)} = \frac{P(A) \cdot P(B|A)/P(B)}{P(\neg A) \cdot P(B|\neg A)/P(B)} = \text{Odds}(A) \cdot \frac{P(B|A)}{P(B|\neg A)} \tag{8.5}$$

Let us define the "odds ratio" of A given B, $\text{OR}(A|B) = \text{Odds}(A|B)/\text{Odds}(A)$; that is, the factor by which learning B affects the odds on A. For instance if $P(A) = 1/3$ and $P(A|B) = 3/4$. then $\text{Odds}(A) = 1/2$, $\text{Odds}(A|B) = 3$ so $\text{OR}(A|B) = 6$; learning B has increased the odds on A by a factor of 6. Then we can rewrite equation 8.5 in the form

$$\frac{P(B|A)}{P(B|\neg A)} = \frac{\text{Odds}(A|B)}{\text{Odds}(A)} = \text{OR}(A|B) \tag{8.6}$$

Now using equation 8.6, we can rewrite equation 8.4 in the form

$$\text{Odds}(X|E, F) = \text{OR}(X|E) \cdot \text{OR}(X]F) \cdot \text{Odds}(X) \tag{8.7}$$

Dividing through by $\text{Odds}(X)$ gives, finally.

$$\text{OR}(X|E, F) = \text{OR}(X|E) \cdot \text{OR}(X|F). \tag{8.8}$$

Returning now to our original problem:
Suppose that $P(X) = 1/3$, $P(X|E) = 0.8$ and $P(X|F) = 0.9$.
Then $\text{Odds}(X) = 1/2$, $\text{Odds}(X|E) = 4$, and $\text{Odds}(X|F) = 9$, so $\text{OR}(X|E) = 8$ and $\text{OR}(X|F) = 18$.
Using the independence assumption, by equation 8.8, $\text{OR}(X|E,F) = \text{OR}(X|E) \cdot \text{OR}(X|F) = 144$.
Therefore $\text{Odds}(X|E,F) = \text{OR}(X|E,F) \cdot \text{Odds}(X) = 72$,
and $P(X|E,F) = \text{Odds}(X|E,F)/(1 + \text{Odds}(X|E,F)) = 72/73 = 0.986$.

For example: In the trial of O.J. Simpson for murdering his ex-wife Nicole Brown and Ronald Goldman, there was evidence that Simpson had abused his wife on earlier occasions, and the question arose as to whether this evidence could be presented. The prosecution argued that the evidence was relevant, because most spousal murders follow earlier abuse. The defense argued that it was irrelevant and merely prejudicial, because most men who abuse their wives do not end up murdering them. From the above analysis, we can see that both arguments are incomplete. The real question is, how much more frequent, in terms of odds update, is spousal murder among the population of spousal abusers than among the general population of married men? (It makes sense to separate by gender here, because the incidence of both abuse and murder of men against women is hugely higher than the reverse.) X here is murder, E is abuse, F is all the rest of the evidence.

The details of the derivation above are not important. What is important is the combination of Bayes' law and independence assumptions for combining evidence; Bayes' law is used to munge the formulas into a state where the independence assumptions can be applied. We will see this again, with wide range of less lurid applications, in section 8.11

8.9.2 Application: Secret sharing in cryptography

Suppose that you have a secret text, which you want to split among n people in such a way that, if all n get together they can reconstruct the secret, but no subset of $n-1$ people can reconstruct the secret or any part of it. For example, the secret is the code to launch the nuclear missiles and you want to make sure that they are not launched unless everyone who is supposed to agree does indeed agree.

Let us first consider the case where the secret is a single bit B. Then carry out the following algorithm:

for $(i = 1$ to $n-1)$ $Q_i \leftarrow$ a random bit;
$Q_n = (B + Q_1 + Q_2 + \ldots + Q_{n-1}) \bmod 2$.

Now tell person i the value of the bit Q_i.

Note that

$$Q_1 + \ldots + Q_n \bmod 2 = Q_1 + \ldots + Q_{n-1} + (Q_1 + \ldots + Q_{n-1} + B) \bmod 2 =$$

$$(Q_1 + Q_1) + (Q_2 + Q_2) + \ldots + (Q_{n-1} + Q_{n-1}) + B \bmod 2 = B$$

So the n participants can reconstruct B by adding up their individual pieces mod 2.

I claim that B is independent of any subset S of size $n-1$ of the Q_i. This is clearly true if S does not contain Q_n, as $Q_1 \ldots Q_{n-1}$ were just randomly chosen bits. Suppose that S does contain Q_n but does not contain Q_i. To simplify the notation let us choose $i = 1$, the other cases are obviously the same.
Now $Q_n = ((Q_2 \ldots Q_{n-1} + B) + Q_1) \bmod 2$.
Since $Q_1 \ldots Q_{n-1}$ are chosen randomly, if you know $Q_2 \ldots Q_{n-1}$, then for either value of B, Q_1 has a 50/50 chance of being 1 or 0. But by the above equation,

if $Q_2 \ldots Q_{n-1} + B = 1 \bmod 2$ then $Q_n = 1 - Q_1$;
and if $Q_2 \ldots Q_{n-1} + B = 0 \bmod 2$ then $Q_n = Q_1$.
Therefore if you have been told the values of $B, Q_2 \ldots Q_{n-1}$ then Q_n has a 50/50 chance of being 0 or 1. But before you were told anything, Q_n likewise had a 50/50 chance of being 0 or 1. Thus That is, Q_n is independent of $B, Q_2 \ldots Q_{n-1}$. By the symmetry of independence, B is independent of $Q_2 \ldots Q_n$.

In short, if you have all n pieces, you can construct B but having any set of $n-1$ pieces gives no information at all about B.

If the secret is a string of k bits, then you can do this for each bit, and hand a bitstring of k random bits to each of the n participants. To reconstruct the secret, add up each place in the bit string mod 2. This is known as "bitwise XOR (exclusive or)"; exclusive OR is the same as addition modulo 2.

Note that the argument does not require any assumptions about the distribution of B. It may be that you start with some external information about the distribution of B; what the argument shows is that you don't learn anything more by finding out $n-1$ of the keys. For the same reason $Q_1 \ldots Q_n$ are not necessarily collectively independent absolutely; if you have external information about B, then that will create a dependency.

In older probability books, the fact that pairwise independence does not imply overall independence is often described as a somewhat annoying anomaly of no practical importance. The moral is that practical importance changes over time.

8.10 Random Variables

A *random variable* is a variable that can have a value within some associated domain of values.

If the domain of values is finite, then each possible value for the random variable constitutes an event, and has a probability. The different values for a single random variable constitute a frame of discernment; that is, exactly one of them must be true, so the sum of their probabilities is equal to 1.

A good way to think about random variables[2] is that a random variable is a dartboard. The different values that the variable can take are marked on the dartboard. Throwing a dart and seeing which area it lands in is the event.

Example 8.4 revisited: You flip a coin three times. This can be described using three random variables F_1, F_2, F_3, one for each flip. Each of these takes values within the set { H, T}. So the pair of events F_1=H and F_1=T form a frame of discernment; so does the pair F_2=H and F_2=T; so does the pair F_3=H and F_3=T.

If you have a finite collection of random variables, then an elementary event is an assignment of one value to each variable. For example $F_1 = \mathrm{H} \wedge F_2 = \mathrm{H} \wedge F_3 = \mathrm{T}$ is one elementary event; $F_1 = \mathrm{T} \wedge F_2 = \mathrm{T} \wedge F_3 = \mathrm{T}$ is another elementary event, and so on. The set of elementary events again forms a frame of discernment. An assignment of a probability to each elementary event is called a *joint distribution* over the random variables. For example, one joint distribution over $\{F_1, F_2, F_3\}$ would be

$$P(F_1 = \mathrm{H}, F_2 = \mathrm{H}, F_3 = \mathrm{H}) = 0.4$$
$$P(F_1 = \mathrm{H}, F_2 = \mathrm{H}, F_3 = \mathrm{T}) = 0.1$$
$$P(F_1 = \mathrm{H}, F_2 = \mathrm{T}, F_3 = \mathrm{H}) = 0.07$$
$$P(F_1 = \mathrm{H}, F_2 = \mathrm{T}, F_3 = \mathrm{T}) = 0.02$$

[2]Thanks to Alan Siegel for this metaphor.

$P(F_1 = \mathrm{T}, F_2 = \mathrm{H}, F_3 = \mathrm{H}) = 0.1$
$P(F_1 = \mathrm{T}, F_2 = \mathrm{H}, F_3 = \mathrm{T}) = 0.03$
$P(F_1 = \mathrm{T}, F_2 = \mathrm{T}, F_3 = \mathrm{H}) = 0.08$
$P(F_1 = \mathrm{T}, F_2 = \mathrm{T}, F_3 = \mathrm{T}) = 0.2$

In the above formulas, we have used commas between events to mean conjunction; this is a standard notation in probability theory. Thus $P(F_1 = \mathrm{H}, F_2 = \mathrm{H}, F_3 = \mathrm{H})$ means $P(F_1 = \mathrm{H} \wedge F_2 = \mathrm{H} \wedge F_3 = \mathrm{H})$; $P(E \mid F, G)$ means $P(E \mid F \wedge G)$ and so on.

As in section 8.7, any event E is the disjunction of elementary events, and $P(E)$ is the sum of the probabilities of these elementary events. For example,

$(F_1 = \mathrm{H} \wedge F_3 = \mathrm{T}) \equiv (F_1 = \mathrm{H} \wedge F_2 = \mathrm{H} \wedge F_3 = \mathrm{T}) \vee (F_1 = \mathrm{H} \wedge F_2 = \mathrm{T} \wedge F_3 = \mathrm{T})$.
So $P(F_1 = \mathrm{H}, F_3 = \mathrm{T}) = P(F_1 = \mathrm{H}, F_2 = \mathrm{H}, F_3 = \mathrm{T}) + P(F_1 = \mathrm{H}, F_2 = \mathrm{T}, F_3 = \mathrm{T})$.

Thus absolute probability of any event can be calculated from the joint distribution. Since $P(E|F) = P(E \wedge F)/P(F)$, any conditional probability can be calculated from absolute probabilities. Therefore *the joint probability distribution determines all absolute and conditional probabilities associated with these random variables.*

Two random variables E and F are *independent* if, for every value u in the domain of E and v in the domain of F, the event $E = u$ is independent of the event $F = v$. That is,
$P(E = u, F = v) = P(E = u) \cdot P(F = v)$.

Notational note: When a relation like the one above holds for all values in the domains of the random variable involved, it is common in probabilistic writings to write the relation purely in terms of the random variable, omitting the values. For instance, the above equation
$P(E = u, F = v) = P(E = u) \cdot P(F = v)$ would be written $P(E, F) = P(E) \cdot P(F)$. This abbreviated form is certainly convenient, but it can also be quite confusing, until you are used to it. I will avoid it in this book, but I mention it since the reader may well see it elsewhere.

In general a probabilistic model consists of

- A choice of random variables.
- A set of independence assumptions. Unless the number of random variables is small, then the dependencies in the model had better be sparse (that is, almost everything must be conditionally or absolutely independent of almost everything else).
- Numerical values for the probabilities involved in the dependency relationships, or methods for obtaining these.

8.11 Application: Naive Bayes classification

In this section we will discuss how Bayes' law and independence assumptions are used in the Naive Bayes method of constructing classifiers from labelled data.

A *classification* problem has the following form: You have a collection of *instances*. For each instance, you are given some information, which can be viewed as values of a set of *predictive attributes*. Your task is to assign the instance to one of another of categories; each category is a possible value of a *classification attribute*. For example:

- Character recognition: An instance is an image of a printed symbol. The predictive attributes are various geometric features of the image. The classification attribute has values which are the various charaters in the character sets; i.e. the space of values is { 'A', 'B', ... }.

  Many other computer vision problems likewise can be formulated as classification problems. In *face recognition,* the values of the classification attribute are different people. In *image labeling* the set of values of the classification attribute is some large vocabulary of categories; e.g. { "building", "human", "car", "tiger", "flower" ... }. In *pornography filtering* (don't snicker; this is a critical task for web browser support) the classification attribute has values { "pornography", "decent" }.

- Medical diagnosis. An instance is a patient. The predictive attributes are test results and features of the medical history. For each disease, there is a classification attribute whose values are "true" or "false".

- Finance. An instance is an applicant for a loan. The predictive attributes are income, assets, collateral, purpose of the loan, previous credit history, and so on. The classification attribute has values "approve" and "disapprove".

- Text classification. An instance is a piece of text. The predictive attributes are the words of the text (or other information about it). The classification attribute is some important characteristic of the text. For instance, in email filtering, the attribute might have values { 'spam', 'ordinary', 'urgent' }. In information retrieval or web search, the classification attribute is set by the query, and has values { 'relevant to query Q', 'irrelevant to query Q' }

A *classifier* is a program or algorithm that carries out a classification task. Most automated classifiers use some form of machine learning from a *labelled corpus* (this is known as *supervised* learning). A labelled corpus is a table of instances where the correct value of the classification attribute is given; for instance a set of images of characters labelled with the actual character, or a set of email messages labelled "spam" or "not spam", and so on. The machine learning task is to use the corpus to construct a classifier that works well. The use of corpus-based machine learning techniques to construct classifiers probably constitutes the majority of work in machine learning, both applied and theoretical.

One way to think about the classification task is to view it probabilistically; we want to find the most *likely* value of the classification attribute given the predictive attributes. That is: We will take the predictive attributes to be random variables $A_1 \dots A_k$ and we will take the classification attribute to be a random variable C. For a new instance $\mathbf{x}$, we are given that the predictive attributes have $a_1 \dots a_k$ and we wish to find the value of c that maximizes $P(C = c | A_1 = a_1, A_2 = a_2 \dots A_k = a_k)$.

We estimate the probability of events by their frequency in the table T of labelled instances. For any event E, let us write $\#_T(E)$ to mean the number of instances of E in table T, and $\text{Freq}_T(E)$ to be the frequency of E in T; thus $\text{Freq}_T(E) = \#_T(E)/\#T$. Likewise, we will write $\text{Freq}_T(E|F) = \#_T(E \wedge F)/\#_T(F)$ Thus we estimate $P(E) \approx \text{Freq}_T(E)$ and $P(E|F) \approx \text{Freq}_T(E|F)$. However this only works if $\#_T(E)$ and $\#_T(E \cap F)$ are not too small. In particular if these are zero, this estimate is pretty useless.

Suppose, for example, there are only two predictive attributes and the table T is large, so every combination $C = c, A_1 = a_1, A_2 = a_2$ has numerous instances in T. Then we can estimate

$$P(C = c | A_1 = a_1, A_2 = a_2) \approx \text{Freq}_T(C = c | A_1 = a_1, A_2 = a_2) = \\ \#_T(C = c, A_1 = a_1, A_2 = a_2)/\#_T(A_1 = a_1, A_2 = a_2)$$

and we are done. However, for the kind of problems we discuss above, there may be hundreds or thousands or more of attributes, and each instance is unique; this particular collection of predictive attributes has *never* before appeared in the table. In that case we cannot use the approximation

function LearnClassifier(**in** T:table; C: attribute): **return** classifier;
{ **for each** (value c of C)
compute $\text{Freq}_T(C = c)$
for each (attribute $A \neq C$ in T)
for each (value a of A)
compute $\text{Freq}_T(A = a, C = c)$
endfor endfor endfor
return a table of all these frequencies (this table is the classifier) }

function ApplyClassifier(**in** Q:classifier, X:unlabelled instance; C: attribute) **return** value of C;
return $\text{argmax}_{c:\text{ value of }C} \text{Freq}_T(C = c) \cdot \Pi_{A:\text{attribute}} \text{Freq}_T(A = X.A|C = c)$

/* In the above expression, $X.A$ denotes the A attribute of instance X.
Π_A means the product over all the different attributes.
$\text{argmax}_c E(c)$ means return the value of c that maximizes the expression $E(c)$ */

Table 8.1: Naive Bayes Algorithm

$$P(C = c|A_1 = a_1 \ldots A_k = a_k) \approx \text{Freq}_T(C = c|A_1 = a_1 \ldots, A_k = a_k) =$$
$$\#_T(C = c, A_1 = a_1 \ldots A_k = a_k)/\#_T(A_1 = a_1 \ldots A_k = a_k),$$

because both numerator and denominator are zero.

Instead, in the Naive Bayes method, we make an independence assumption; as it happens, a very similar one to the one we made in section 8.9.1. We assume that the predictive attributes are all conditionally independent given the classification attribute. Having done that, we can now proceed as follows:

$$P(C = c|A_1 = a_1 \ldots A_k = a_k) = \quad \text{(by Bayes's law)}$$
$$P(C = c) \cdot P(A_1 = a_1 \ldots A_k = a_k|C = c)/P(A_1 = a_1 \ldots A_k = a_k) = \quad \text{(by the independence assumption)}$$
$$P(C = c) \cdot P(A_1 = a_1|C = c) \cdot \ldots \cdot P(A_k = a_k|C = c)/P(A_1 = a_1 \ldots A_k = a_k)$$

However since what we are looking for is the value of c that maximizes this expression, and since c does not appear in the denominator, we can ignore the denominator. The denominator is just a normalizing expression; without it, we have an equivalent unnormalized set of weights. So our problem now is to find c that maximizes $P(C = c) \cdot P(A_1 = a_1|C = c) \cdot \ldots \cdot P(A_k = a_k|C = c)$. But now (hopefully) all of these probabilities can be estimated from frequencies in the table, as long as the table is large enough that the pair $A_i = a_i, C = c$ is represented reasonably often for each value of a_i and c. So we estimate

$$P(C = c) \cdot P(A_1 = a_1|C = c) \cdot \ldots \cdot P(A_k = a_k|C = c) \approx$$
$$\text{Freq}_T(C = c) \cdot \text{Freq}_T(A_1 = a_1|C = c) \cdot \ldots \cdot \text{Freq}_T(A_k = a_k|C = c).$$

Thus, we have the two simple algorithms shown in table 8.1 : one to learn the classifier Q for classification attribute C from the table T of labelled data, the other to apply the classifier to a new instance X.

For example, let us take the case of email classification. One way to apply Naive Bayes[3] is to take every word that appears in the table to be a predictive attribute of a message: "Hi" is one attribute,

[3]There are a number of different ways to apply Naive Bayes to text classification; the one described here, called the Bernoulli model, fits most neatly into our schema.

and "conference" is another attribute and "OMG" is another attribute, and so on. The attributes are Boolean; attribute W of message M is true if W appears in M and false otherwise. So the three numbers $\text{Freq}_T(\text{“}conference'' = true|C = spam)$, $\text{Freq}_T(\text{“}conference'' = true|C = ordinary)$, and $\text{Freq}_T(\text{“}conference'' = true|C = urgent)$ are the fractions of spam / ordinary / urgent messages that contain the word "conference". Since (in my email) "conference" appears much more frequently in ordinary messages than in either spam or urgent messages, if it appears in a new message, it will give a much stronger vote for considering this new message to be ordinary than to be either spam or urgent.

There are two problems here; one technical and one fundamental. The technical problem is that this application does not support the hopeful assumption mentioned above that every pair of a value of a predictive attribute with a value of the classification attribute appears some reasonable number of times in the table. We have too many predictive attributes. If an instance contains an attribute value $A_i = a_i$ that has never appear together with some classification value $C = c$ in the table, then the factor $\text{Freq}_T(A_i = a_i|C = c)$ is equal to zero, and therefore the product will be equal to zero, whatever other evidence is present. For example, I have never received an urgent message containing the word "Newfoundland"; therefore $\text{Freq}_T(\text{“}Newfoundland'' = true|C = urgent) = 0$. But if I now receive the email

> URGENT: You must get me the information you promised me a month ago ASAP. This is vitally important. I need it today, because I'm going to a funeral in Newfoundland tomorrow.

then I would want the classifier to notice the words "URGENT", "ASAP", "vitally" and "important" and classify this as urgent, rather than saying that, because it contains the word "Newfoundland" it can't possibly be urgent.

This is known as the *sparse data problem;* it is a common problem in deriving probabilistic models from data. The solution here is to replace zero values by values that are small but non-zero; this is called smoothing. But of course, we can't treat zero values as better than a very small non-zero values, so we have to move up all small values. The usual solution, known as the Laplacian correction, is to use an estimate of the form $P(A = a|C = c) = (\text{Freq}_T(A = a|C = c) + \epsilon)/(1 + N\epsilon)$ where N is the number of possible values of A and $\epsilon > 0$ is a small parameter.

The fundamental problem is that the independence assumption bears no relation to reality. It is not remotely true that the predictive attributes are conditionally independent given the classification attribute. "Conference" is associated with "proceedings" and "paper" and "deadline" and "hotel"; and "meeting" is associated with "agenda" and "minutes" and "report"; and "late", "husband", "million", "unable", "collect", "account", "number" and names of various foreign countries go together; as do "Viagra" and — well, fill that one in for yourself.

The use of independence assumptions that have no basis in reality is characteristic of applied probabilistic models generally and of naive Bayes in particular; that is why it is called "naive". One clear consequence in naive Bayes applications is that the computed probabilities tend to be much too one-sided; that is to say, the classifier assigns a much higher confidence to its predictions than its actual accuracy warrants. Essentially, the naive Bayes takes as independent evidence what is actually just the same piece of evidence repeated a number of times. Nonetheless, in many applications, naive Bayes gives answers of a very good quality, computed quite cheaply.

A couple of further technical observations about the naive Bayes algorithm. In practice, rather than multiply the frequencies, it is common to add the logs of the frequencies. Thus

$$\log(P(C = c|A_1 = a_1 \dots A_k = a_k)) =$$

$$\log(\underset{T}{\text{Freq}}(C = c) \cdot \underset{T}{\text{Freq}}(A_1 = a_1|C = c) \cdot \dots \cdot \underset{T}{\text{Freq}}(A_k = a_k|C = c)) =$$

$$\log(\underset{T}{\text{Freq}}(C = c)) + \log(\underset{T}{\text{Freq}}(A_1 = a_1|C = c)) + \ldots + \log(\underset{T}{\text{Freq}}(A_k = a_k|C = c))$$

This has two advantages. First multiplying a long list of numbers between 0 and 1 (often mostly rather small numbers) results in underflow rather quickly; the use of the logarithm avoids this.

Second, this formulation demonstrates that the naive Bayes classifier has a simple, and familiar, form; it is just a linear discriminator. Define a vector space with one dimension for each value of each predictive attribute; that is, for each attribute A and for each possible value v there is a separate dimension $d(A, v)$. Let n be the number of such i dimensions. For each value c of the classification attribute, define $\vec{w}_c$ in $\mathbb{R}^n$ such that $\vec{w}[d(A, v)] = \log(\text{Freq}_T(A = v|C = c))$, and define a real quantity $t_c = \log(\text{Freq}_T(C = c))$. With any instance x associate a Boolean vector $\vec{x}$ in $\mathbb{R}^n$ such that $\vec{x}[d(A, v)] = 1$ if $x.A = v$ and $\vec{x}[d(A, v)] = 0$ if $x.A \neq v$. Then when the classifier classifies an instance $\vec{x}$, it simply computes the value of the expression $t_c + \vec{w}_c \cdot \vec{x}$ for each category c, and it picks the value of c for which this expression is largest.

Finally a comment about running time. Generally in machine learning, the learning part is executed separately from the actual task execution. The learning part is said to be "offline"; it is allowed to run quite slowly. The task executor that it creates is usually what the end user is interacting with; it is require to run quickly, "online". The two running times are considered separately. In the case of naive Bayes, the learning algorithm goes through the table T and generates the vectors $\vec{w}_c$ and the quantities t_c above; this can be implemented to run in time $O(|T|)$ where $|T|$ is the size of the table. The classifier computes the value of $t_c + \vec{w}_c \cdot \vec{x}$ for each value of c; this runs in time $O(kc)$ where k is the number of attributes and c is the number of possible values for the classification attribute. In the case where $\vec{x}$ is sparse, as in text classification, it runs in time $c \cdot NZ(\vec{x})$ where $NZ(\vec{x})$ is the number of non-zero elements. So the learning algorithm runs reasonably quickly, and the classifier runs extremely quickly.

Exercises

Exercise 8.1

Let Ω be the sample space with 6 elements, $\Omega = \{a, b, c, d, e, f\}$. Let P be the following probability distribution:

$$P(a) = 0.05.\ P(b) = 0.1.\ P(c) = 0.05.\ P(d) = 0.1.\ P(e) = 0.3.\ P(f) = 0.4.$$

Consider the events $X = \{a, b, c\}$; $Y = \{b, d, e\}$, $Z = \{b, e, f\}$.

Evaluate the following

A. $P(X)$.

B. $P(Y)$.

C. $P(Z)$.

D. $P(X, Y)$.

E. $P(X|Y)$.

F. $P(X|Z)$.

G. $P(Y|Z)$.

H. $P(Y|X,Z)$.

I. $P(X,Y|Z)$.

I. Are X and Y absolutely independent?

J. Are X and Z absolutely independent?

K. Are X and Y conditionally independent given Z?

Exercise 8.2

Let A,B,C,D,E be five Boolean random variables. Assume that you are given the following independence assumptions:

> A and B are independent absolutely. D is conditionally independent of both A and C given B. E is conditionally independent of A, B, and D given E.

You are given the following probabilities:

P(A=T) = 0.9.	P(A=F) = 0.1.
P(B=T) = 0.6.	P(B=F) = 0.4
P(C=T|A=T,B=T) = 0.9.	P(C=F|A=T,B=T) = 0.1.
P(C=T|A=T,B=F) = 0.8.	P(C=F|A=T,B=F) = 0.2.
P(C=T|A=F,B=T) = 0.4.	P(C=F|A=F,B=T) = 0.6.
P(C=T|A=F,B=F) = 0.1.	P(C=F|A=F,B=F) = 0.9.
P(D=T|B=T) = 0.8.	P(D=F|B=T) = 0.2
P(D=T|B=F) = 0.2.	P(D=F|B=F) = 0.8
P(E=T|C=T) = 0.1.	P(E=F|C=T)=0.9.
P(E=T|C=F) = 0.8.	P(E=F|C=F)=0.2.

Compute the following probabilities (you may use MATLAB).

A. P(A=T,B=T)

B. P(A=T $\vee$ B=T) (either A or B or both are T).

C. P(C=T)

D. P(C=T|A=T)

E. P(C=T,D=T)

F. P(A=T|C=T)

G. P(A=T|B=T,C=T)

H. P(E=T|A=T)

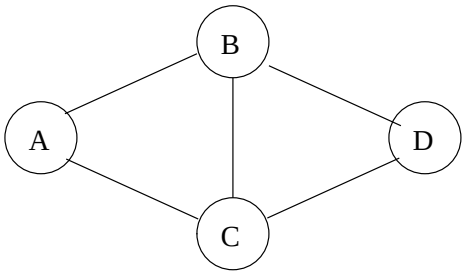


Figure 8.1: Network

Exercise 8.3

A. Given that $P(E) = 1/2$, $P(E|F) = 3/4$, $P(E|G) = 4/5$, and assuming that F and G are independent evidence for E (that is, they are conditionally independent given E and given $\neg E$), what is $P(E|F, G)$?

B. Construct a joint probability distribution over E, F, G such that $P(E) = 1/2$, $P(E|F) = 3/4$ $P(E|G) = 4/5$ but $P(E|F, G) = 1/10$.

Exercise 8.4

Suppose that you have a coin that comes up heads with probability 3/4, and you flip it three times. For $i = 1 \ldots 3$, let F_i be the Boolean random variable which is true if the ith flip comes up heads. Let C be the random variable with values 0,1,2,3 which is the total number of heads in the three flips.

A. What is the associated sample space Ω? What is the probability distribution P over Ω?

B. What is the probability distribution of C?

C. What is the conditional probability distribution of F_1 given that $C = 1$?

D. Are F_1 and F_2 conditionally independent given that $C = 1$?

Exercise 8.5

Figure 8.1 shows a network with four nodes and five edges. Suppose that each connection fails with probability 1/10 and that failures of connections are all independent events.

A. What is the probability that there is an active path from B to C? Hint: There are no active paths from B to C if all three paths B-A-C, B-C, and B-D-C have failed; and these are independent events.

   This is known as a *series-parallel decomposition*.

B. What is the probability that there is a path from node A to D?

   Hint: In this case it is not possible to do a series-parallel decomposition, and it is very easy, unless one is systematic, to miss a case. Rather, there are 32 elementary events i.e. assignments of "working" or "failing" to each of the five edges. You should begin by enumerating all 32, implicitly or explicitly.

C. What is the probability that there is an active path between all pairs of nodes?

Exercise 8.6

(You may use MATLAB.) In example 8.5 (p. 199), we computed the number of 5 card poker hands, and the probability that a random hand is a flush.

A. How many different hands are straights (numbers in sequence; suits arbitrary)? What is the probability that a random hand is a straight?

B. How many hands are straight flushes (both a straight and a flush)? What is the probability that a random hand is a straight flush? Are the two events "straight" and "flush" independent?

C. (More difficult) Suppose that two hands are dealt. Given that the first is a flush, what is the probability that the second is also a flush? Are the two events "the first hand is a flush" and "the second hand is a flush" independent?

Problems

Problem 8.1

Prove axioms P.1–P.4 from axioms F.1, F.2.

Problem 8.2

(Difficult) Prove theorem 8.2.

Programming Assignments

Assignment 8.1

Write two MATLAB functions `SplitSecret(S,N)` and `RecoverSecret(Q)` that implement the secret-sharing technique described in section 8.9.2. Specifically, `SplitSecret(S,N)` takes as argument a character string `S` and a number `N`. It returns an $\texttt{N} \times |\texttt{S}|$ array `Q` of 1's and 0's, where each row is the part of the secret given to one of the sharers. `RecoverSecret(Q)` takes this matrix `Q` as input and computes the string `S`.

Assignment 8.2

Generalize exercise 8.5.C as follows. Write a function `ProbConnect(P)` which computes the probability that all nodes are connected in a network where the probability that the node from `I` to `J` is active is given by `P[I,J]`. That is: `P` is an $\texttt{N} \times \texttt{N}$ matrix where `P[I,J]` is the probability that the arc from `I` to `J` is working (connections may not be symmetric). If `P[I,J]=0` then there is no connection from `I` to `J`. Assume that each arc is independent of all the others.

For instance, in the particular example considered in exercise 8.5, `P` would be the matrix

$$P = \begin{bmatrix} 0 & 0.1 & 0.1 & 0 \\ 0.1 & 0 & 0.1 & 0.1 \\ 0.1 & 0.1 & 0 & 0.1 \\ 0 & 0.1 & 0.1 & 0 \end{bmatrix}$$

You should just implement this in the naive way; enumerate all 2^E ways to label the arcs working and non-working (E is the number of non-zero edges), and for each one, calculate its probability. (There are certainly more efficient algorithms than this, but all known algorithms are exponential in the worst case.)

Assignment 8.3

Consider the following simplified variant of the card game "Blackjack". Two players are alternately dealt cards, which are random integers between 1 and 10, one at a time. (Assume that each deal is independent; the numbers are dealt by rolling a 10-sided die, not by dealing from a finite deck.) At each stage, a player may either request a card, or may pass and not get assigned a card. If a player's total is exactly 21, he immediately loses. If a player's total exceeds 21, then he immediately loses. If a player has passed on one round, he is permitted to continue drawing cards on later rounds. If both players have passed, then the player with the higher total wins. In the case of a tie, the first player to pass wins.

For instance, consider the following sequences with two players:

Sequence 1:

Player A draws 8.
Player B draws 3.
Player A draws 7.
Player B draws 5.
Player A draws 8, and loses (exceeds 21).

Sequence 2:

Player A draws 8.
Player B draws 3.
Player A draws 9.
Player B draws 7.
Player A passes.
Player B draws 9.
Player A draws 3.
Player B draws 7 and loses (exceeds 21).

We now generalize the above in two ways. First, the number of card values `NCards` may be different from 10. Second, instead of a single target value 21, we have a target range, from `LTarget` to `UTarget`. If the player reaches a total between `LTarget` and `UTarget`, inclusive, he immediately wins. If the player's total exceeds `UTarget`, he immediately loses.

The optimal strategy can be computed using a dynamic programming implementation of a probabilistic calculation. First, we note the following:

A. If it is player X's turn to play, then his optimal move is determined by a game state consisting of three parts: Whether or not the player Y has just passed, X's total points, and Y's total points.

B. If Y did not pass on the previous turn, and X's total is less than Y's, then X should definitely draw, because if he passes, Y can immediately win.

C. It will never happen that the game ends with both players passing, because whichever player would lose will do better to take a chance on drawing.

In view of these observations, the optimal strategy and the player's chances of winning in any given situation can be expressed in two arrrays, of size $(\texttt{LTarget}-1)\times(\texttt{LTarget}-1)$. The Boolean array `Play[XT,YT]` gives the optimal move for player X in the case where player Y did not pass on the previous move, where `XT` and `YT` are the current totals for X and Y: `Play[XT,YT]=1` if X should draw, 0 if he should pass. The array `Prob[XT,YT]` is the probability that X will win if he makes the recommended move.

The assignment, then, is to write a function `Blackjack(NCards,LTarget,UTarget)` returning the two arrays `Play` and `Prob`.

The two arrays are filled in together working backward, from the game's end to its beginning. For instance, if `LTarget = 21` the algorithm computes first `Prob[20,20]` and `Play[20,20]`; then `[19,20]` and `[20,19]`; then `[18,20]`, `[19,19]`, and `[20,18]`; and so on.

The value of the two arrays is filled in as follows:

```
if (rules B or C determine the winning move)
      then compute the probability for that move
      else compute the probabilities for both moves
              and use the move with higher probability;
save the move in Play[XT,YT] and the probability in Prob[XT,YT].
endif
```

The probability that X will win if he draws in state XT,YT can be computed by considering each possible deal. If X draws a card with value CARD and neither wins nor loses, then it will be Y's turn, and Y will be in the state $\langle YT, XT+CARD\rangle$ The probability that Y wins in that state is `Prob[YT,XT+CARD]`; hence the probability that X wins if Y is in that state is `1−Prob[YT,XT+CARD]`.

```
Computing the probability that X will win if he draws in state XT,YT:
{ ProbWinning = 0.0
  for (CARD=1:NCards) {
     if (XT+CARD > UTarget) then ProbYWins = 1;
       elseif (XT+CARD >= LTarget) then ProbYWins = 0;
       else ProbYWins = Prob[YT,XT+CARD];
     ProbWinning = ProbWinning + (1-ProbYWins)/NCards;
  endfor
  return ProbWinning
}
```

The probability that X will win if he passes after Y drew on the previous turn is

```
 if (YT > XT) then 0
 else 1-Prob[YT,XT]
```

Chapter 9

Numerical Random Variables

Random variables whose domain is a set of numbers are important in a wide range of applications. Most of mathematical probability theory deals the properties of numerical random variables.

Example 8.2, revisited: You roll a fair die. The random variable D has domain $\{1, 2, 3, 4, 5, 6\}$. It is uniformly distributed, so $P(D = x) = 1/6$ for each value x.

Example 9.1: On May 5, 2010, you poll 1000 randomly chosen Americans as to their opinion of President Obama. Let us say that the question is Boolean: favorable or unfavorable. We can define a numerical random variable X whose value is the number of people in the poll who answer "favorable". The domain of the random variable is $\{0, 1, \ldots 1000\}$. We will discuss the probability function in section 9.6.2. Assuming that we are careful not to ask the same person twice, then this is an instance of *sampling without replacement*, discussed in example 8.7.

Most numerical random variables have a domain which is in one of three categories:

A. The domain is a finite set of numbers.

B. The domain is an infinite set of integers.

C. The domain is the real line, or an interval in the real line.

In this chapter, we will begin with category (A); we will introduce category (B), which is not very different, in section 9.5. We will discuss category (C), which is substantially different from (A) or (B), in section 9.7.

The fundamental concepts and properties of numerical random variables are largely the same for all three categories, so we will introduce them here in the simplest context of random variables with finite domains. The first concept is the idea of a function of a random variable. If X is a random variable and f is a function over the domain of X, then $f(X)$ is also a random variable; the value of $f(X)$ is always f applied to the value of X. Likewise, if $X_1 \ldots X_k$ are random variables, and $f(x_1 \ldots x_k)$ is a function of k arguments, then $f(X_1 \ldots X_k)$ is a random variable. Therefore, the event $f(X_1 \ldots X_k) = c$ is the union of the events $f(X_1 = d_1 \ldots X_k = d_k)$ over all tuples $\langle d_1 \ldots d_k \rangle$ for which $f(d_1 \ldots d_k) = c$.

Example 8.2, revisited: As above, let D be the result of rolling a fair die. Then $E = D + 1$ is a random variable; the domain of E is $\{2, 3, 4, 5, 6, 7\}$, and it is uniformly distributed. Moreover, the value of E is tied to the value of D. For example

$$P(E = 3 \mid D = 2) = 1.$$

$$P(E = 3 \mid D = 3) = 0.$$

Example 9.2: You roll two fair dice. There are two random variables: D_1 for the first roll, D_2 for the second. Each is uniformly distributed and the two random variables are independent. Therefore, for each pair of values u, v, $P(D_1 = u, D_2 = v) = P(D_1 = u) \cdot P(D_2 = v) = (1/6) \cdot (1/6) = 1/36$.

Let $S = D_1 + D_2$. S is a random variable with domain $\{2, 3, \ldots 12\}$. The probability that $S = w$ is equal to the sum of $P(D_1 = u, D_2 = v)$ over all u, v such that $u + v = w$. For instance

$$P(S = 3) = P(D_1 = 1, D_2 = 2) + P(D_1 = 2, D_2 = 1) = 2/36 = 1/18$$

$$P(S = 4) = P(D_1 = 1, D_2 = 3) + P(D_1 = 2, D_2 = 2) + P(D_1 = 3, D_2 = 3) = 3/36 = 1/12$$

Thus, S is *not* uniformly distributed.

Note that S is not the same as the random variable $F = D_1 + D_1$. F has the domain $\{2, 4, 6, 8, 10, 12\}$ and is uniformly distributed over that range. $P(F = 4|D_1 = 2) = 1$ whereas $P(S = 4|D_1 = 2) = 1/6$. This illustrates that D_1 and D_2 are two *different* random variables, though they have identical domain and probability distribution.

The following is trivial but useful.

Theorem 9.1. *If X and Y are independent random variables, function f is a function over the domain of X and g is a function over the domain of Y, then $f(X)$ and $g(Y)$ are independent.*

Proof: Let u be a value of $f(X)$ and let v be a value of $g(Y)$. Let $A = f^{-1}(u) = \{a|u = f(a)\}$, the set of all values a that f maps into u; and let $B = g^{-1}(v) = \{b|v = g(b)\}$, the set of all values b that g maps into v. Then

$$P(f(X) = u, g(Y) = v) = P(X \in A, Y \in B) = \sum_{a \in A, b \in B} P(X = a, Y = b) =$$

$$\sum_{a \in A, b \in B} P(X = a) \cdot P(Y = b) = [\sum_{a \in A} P(X = a)] \cdot [\sum_{b \in B} P(Y = b)] =$$

$$P(X \in A) \cdot P(Y \in B) = P(f(X) = u) \cdot P(g(Y) = v)$$

∎

9.1 Marginal distribution

Suppose that you have two random variables (not necessarily numeric): X with domain $\{u_1 \ldots u_m\}$ and Y with domain $\{v_1 \ldots v_n\}$. You can then construct a $m \times n$ matrix M where $M[i, j] = P(X = u_i, Y = v_j)$. If you sum up each row, you get a column vector of length m; this is the overall probability distribution over X. If you sum up each row, you get a row vector of length n; this is the overall probability distribution over Y. These are known as the marginal distributions over the table, because you write them in the right and bottom margins. Table 9.1 shows an example, where X has domain { a,b,c,d } and Y has domain { e,f,g,h }

The proof that this works is simple. We illustrate using the above example: The event $Y = f$ is equivalent to the disjunction $(Y = f \wedge X = a) \vee (Y = f \wedge X = b) \vee (Y = f \wedge X = c) \vee (Y = f \wedge X = d)$. Therefore

$$P(Y = f) = P(Y = f, X = a) + P(Y = f, X = b) + P(Y = f, X = c) + P(Y = f, X = d)$$

The general case is exactly analogous, so we have the following theorem:

X\Y	e	f	g	h	P(X)
a	0.01	0.05	0.10	0.03	0.19
b	0.20	0.02	0.06	0.02	0.30
c	0.08	0.08	0.04	0.02	0.22
d	0.01	0.07	0.11	0.10	0.29
P(Y)	0.30	0.22	0.31	0.17	

For instance $P(X{=}\text{a}, Y{=}\text{g}) = 0.10$. $P(X{=}\text{b}) = 0.30$. $\text{P}(Y{=}\text{f}) = 0.22$.

Table 9.1: Marginal distribution

Theorem 9.2. *Let X and Y be random variables and let u be a value of X. Then $P(X = u) = \sum_v P(X = u, Y = v)$.*

9.2 Expected value

The *expected value* of a random variable X, denoted $\text{Exp}(X)$, also called the *mean* of X, is the weighted average of possible outcomes, where each outcome is weighted by the probability that it will occur.

$$\text{Exp}(X) = \sum_v v \cdot P(X = v)$$

Note that $\text{Exp}(X)$ is not a random variable; it is just a number.

For instance if D is the random variable for the roll of a fair die, then

$$\text{Exp}(D) = 1 \cdot P(D = 1) + 2 \cdot P(D = 2) + 3 \cdot P(D = 3) + 3 \cdot P(D = 4) + 5 \cdot P(D = 5) + 6 \cdot P(D = 6) =$$

$$(1 \cdot 1/6) + (2 \cdot 1/6) + (3 \cdot 1/6) + (4 \cdot 1/6) + (5 \cdot 1/6) + (6 \cdot 1/6) = 21/6 = 7/2$$

Example 9.2 revisited: Let X be the roll of an unfair coin that comes up heads 3/4 of the time, and let us associate the value 1 with heads and the value 0 with tails.
Then $\text{Exp}(X) = 1 \cdot P(X = 1) + 0 \cdot P(X = 0) = 3/4$.

Suppose that the possible values of X are $v_1 \ldots v_k$ with associated probabilities $p_1 \ldots p_k$. Define the vectors $\vec{v} = \langle v_1 \ldots v_k \rangle$ and $\vec{p} = \langle p_1 \ldots p_k \rangle$. Then $\text{Exp}(X) = \vec{v} \cdot \vec{p}$.

Clearly for any constant c, $\text{Exp}(X + c) = \text{Exp}(X) + c$ and $\text{Exp}(c \cdot X) = c \cdot \text{Exp}(X)$.

Expected value satisfies the following simple and important theorem.

Theorem 9.3. *Let X and Y be random variables. Then* $\text{Exp}(X + Y) = \text{Exp}(X) + \text{Exp}(Y)$.

What is remarkable about this theorem is that it does *not* require that X and Y be independent. That means that it can be applied in cases where determining the distribution of $X+Y$ and carrying out the summation is difficult.

For example, consider the problem of sampling without replacement. Suppose that there is an urn with r red balls and b black balls, and you choose a sample of s balls without replacement. Let Q be the random variable which is the number of red balls in the sample. What is $\text{Exp}(Q)$? To do this directly, we would have to find the distribution of Q, which we will do in section 9.6.2 and then we would have to perform the summation $\sum_{i=0}^{r+b} i \cdot P(Q = i)$. It can be done, but it takes some work

and some combinatorics. But we can avoid all that just by using theorem 9.3. Define the numerical random variables $Q_1 \ldots Q_s$ as follows:

$Q_i = 1$ if the ith ball in the sample is red.
$Q_i = 0$ if the ith ball in the sample is black.

A priori, each ball in the urn has an equal shot of being chosen as the ith ball. Therefore $P(Q_i = 1) = r/(r+b)$ and $P(Q_i = 0) = b/(r+b)$, so $\text{Exp}(Q_i) = 1 \cdot r/(r+b) + 0 \cdot b/(r+b) = r/(r+b)$. Clearly $Q = Q_1 + \ldots + Q_s$, so by theorem 9.3,

$$\text{Exp}(Q) = \text{Exp}(Q_1) + \ldots + \text{Exp}(Q_s) = sr/(r+b)$$

This makes sense: the fraction of balls that are red is $r/(r+b)$ so in a sample of s balls, you would expect that about $(r/(r+b)) \cdot s$ would be red. As discussed in section 8.9, the variables Q_i are not independent, but theorem 9.3 can nonetheless be applied.

For example, in the case of the Obama poll, suppose the total population is z and the fraction of the population supporting Obama is f. We will represent the pro-Obama faction as red balls and the antis as black balls, so $r = fz$ and $b = z - fz$. So if N is the random variable representing the number of people who approve Obama in a poll of 1000, then $\text{Exp}(N) = 1000fz/z = 1000f$.

We can get the same result in a different way. Number the red balls $1 \ldots r$, and define the random variables $X_1 \ldots X_r$ as follows:

$X_i = 1$ if ball i is in the sample.
$X_i = 0$ if ball i is not in the sample.

Since the sample is a random selection of s balls out of $r+b$ total balls, each ball i has probability $P(X_i = 1) = s/(r+b)$ of being chosen for the sample. Therefore $\text{Exp}(X_i) = s/(r+b)$. Clearly $Q = X_1 + \ldots + X_r$ so $\text{Exp}(Q) = \text{Exp}(X_1) + \ldots + \text{Exp}(X_r) = sr/(r+b)$.

Having demonstrated the usefulness of theorem 9.3, let us now prove it. The proof just involves rearranging the order of summation and using marginal probabilities. In the formula below, the summation over u ranges over the domain of X and the summation over v ranges over the domain of Y.

Proof of theorem 9.3:

$$\text{Exp}(X+Y) = \sum_{u,v}(u+v) \cdot P(X=u, Y=v) = \sum_{u,v} u \cdot P(X=u, Y=v) + \sum_{u,v} v \cdot P(X=u, Y=v) =$$

$$\sum_u \sum_v u \cdot P(X=u, Y=v) + \sum_v \sum_u v \cdot P(X=u, Y=v) =$$

$$\sum_u u \cdot (\sum_v P(X=u, Y=v)) + \sum_v v \cdot (\sum_u \cdot P(X=u, Y=v)) = \text{ using marginal summation}$$

$$\sum_u u \cdot P(X=u) + \sum_v v \cdot P(Y=v) = \text{Exp}(X) + \text{Exp}(Y) \qquad \blacksquare$$

The conditional expected value of random variable X given event E is the expected value computed using probabilities conditioned on E: $\text{Exp}(X \mid E) = \sum_v v \cdot P(X = v \mid E)$.

There is a similar theorem for the product of X and Y, *but only if X and Y are independent.*

Theorem 9.4. *If X and Y are independent, then* $\text{Exp}(X \cdot Y) = \text{Exp}(X) \cdot \text{Exp}(Y)$.

Proof: This is just the independence assumption combined with the distributive law.

$\text{Exp}(X \cdot Y) = \sum_{u,v}(u \cdot v) \cdot P(X = u, Y = v) =$ (by independence of X and Y)
$\sum_{u,v}(u \cdot v) \cdot P(X = u) \cdot P(Y = v) =$ (by the distributive law)
$(\sum_u u \cdot P(X = u)) \cdot (\sum_v v \cdot P(Y = v)) = \text{Exp}(X) \cdot \text{Exp}(Y)$. ∎

Suppose that random variable X represents the outcome of a random process which you can run repeatedly in independent trials, and suppose that you run the process N times where N is a large number. Let $S = \langle s_1 \ldots s_N \rangle$ be the sample of output values. Then with very high probability each value v appears approximately $N \cdot P(X = v)$ times in the sample. Therefore, with high probability, the total value of S is $\sum_v v \cdot (N \cdot P(X = v))$, so the average value of elements in S is $\text{Exp}(X)$.

9.3 Decision theory

Decision theory is the application of probability theory to the choice of action. The fundamental premise is that an agent should choose the action, or the strategy, that maximizes the expected value of the *utility* of the outcome. (Utility in this sense is a measure of the goodness of an outcome, on some kind of numeric scale.) This is known as the *maximum expected utility* principle.

Let us start with a simple example. You have the opportunity of buying a lottery ticket. The ticket costs $1. If it is the winning ticket, it will pay $100; otherwise, it will pay nothing. The probability that the ticket will win is 1/1000.

We can analyze this as follows. You have two possible actions:

A.1 To buy a ticket.

A.2 To hold onto your money. (In decision theory, doing nothing is a form of action.)

If you carry out action A.1, then there is a probability of 999/1000 that you will end up $1 poorer and a probability of 1/1000 that you will end up $99 richer. Your *expected gain* is therefore $(999/1000) \cdot -1 + (1/1000) \cdot \$99 = -0.9$. Another way to look at this is that if you buy N tickets where N is a large number, all of which have these same terms and all of which are independent, then with high probability you will end up poorer by $0.9N$.

On the other hand, if you carry out action A.2 then with certainty your gain is zero, so your expected gain is 0. Therefore, A.2 is the preferred action.

Another example: suppose that a student has class in an hour, and has two choices for spending the next hour: (a) Studying for the pass/fail quiz at the start of class; (b) Playing a video game. Suppose that:

- The video game is worth 10 utils (the unit of utility) of enjoyment.
- The activity of studying is worth −5 utils of enjoyment.
- Passing the exam is worth 4 utils.
- Failing the exam is worth −20 utils.

- The net utility is the sum of the utility associated with the next hour's activity plus the utility associated with the result of the exam. (One chooses the action on the basis of the net utility. This is generally taken to be the sum of the utility of the component parts, but there is no logical necessity for this to hold.)
- If the student studies, the probability is 0.75 that he will pass.
- If the student does not study, the probability is 0.5 that he will pass.

Putting this together, if he studies, then there is a 0.75 probability of a net utility of $4 + (-5) = -1$ and a 0.25 probability of a net utility of $4 + (-20) = -16$; so the expected net utility is $0.75 \cdot -1 + 0.25 \cdot -16 = -4.75$. If he doesn't study then there is a 0.5 probability of a net utility of $10 + 4 = 14$ and a 0.5 probability of a net utility of $10 + (-20) = -10$; so the expected net utility is $0.5 \cdot 14 + 0.5 \cdot -10 = 2$. So the rational choice is to play the video game.

9.3.1 Sequence of actions: Decision trees

In a more complex situation, an agent may have to carry out a sequence of actions, and the choice of later actions may depend on the earlier actions.

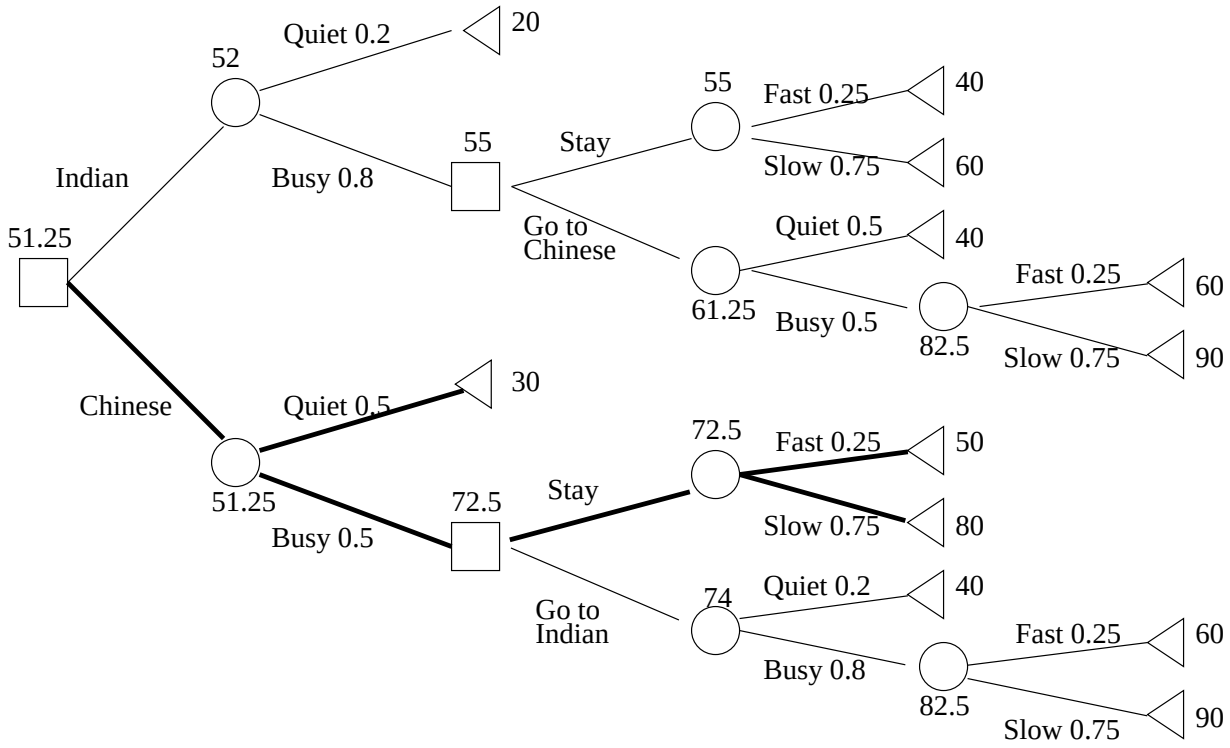
For example, Joe wants to eat lunch out and get back to the office as quickly as possible. There is a Indian restaurant 5 minutes walk north of him and a Chinese restaurant 10 minutes south of him. Either restaurant is in one of two states, quiet or busy, throughout the lunch hour. The Chinese restaurant is busy with probability 0.5; the Indian restaurant is busy with probability 0.8; and these two states are independent events, and do not change throughout the lunch hour. At both restaurants, if the restaurant is quiet, then lunch takes 10 minutes; if the restaurant is busy, then with probability 0.25 lunch will take 30 minutes and with probability 0.75 lunch will take 60 minutes. Assume that Joe's measure of utility is the total elapsed time before he gets back to the office.

Clearly, there are four plans that are worth considering:

1. John walks to the Indian restaurant, and stays there whether or not it is busy. The probability is 0.2 that lunch will take 10 minutes for a total elapsed time of 20 minutes; the probability is $0.8 \cdot 0.25 = 0.2$ that lunch will take 30 minutes for a total elapsed time of 40 minutes; and the probability is $0.8 \cdot 0.75 = 0.6$ that lunch will take 60 minutes for a total elapsed time of 70 minutes. Thus, the expected time is $0.2 \cdot 20 + 0.2 \cdot 40 + 0.6 \cdot 70 = 54$ minutes.
2. John walks to the Indian restaurant. If it is busy, he then walks to the Chinese restaurant. He stays there, whether or not it is busy. The expected time is $0.2 \cdot 20 + 0.8 \cdot 0.5 \cdot 40 + 0.8 \cdot 0.5 \cdot 0.25 \cdot 60 + 0.8 \cdot 0.5 \cdot 0.75 \cdot 90 = 53$ minutes. (Note that the total walking time to go from the office to one restaurant to the other to the office is 30 minutes.)
3. John walks to the Chinese restaurant, and stays there whether or it is busy. The expected time is $0.5 \cdot 30 + 0.5 \cdot 0.25 \cdot 50 + 0.5 \cdot 0.75 \cdot 80 = 51.25$ minutes.
4. John walks to the Chinese restaurant. If it is busy, he walks to the Indian restaurant. He stays there, whether or not it is busy. The expected time is $0.5 \cdot 30 + 0.5 \cdot 0.2 \cdot 40 + 0.5 \cdot 0.8 \cdot 0.25 \cdot 60 + 0.5 \cdot 0.8 \cdot 0.75 \cdot 90 = 52$ minutes.

Therefore the optimal plan is (3).

The situation can be illustrated in a *decision tree*. A decision tree is a tree of the following structure:



Squares — decision nodes.
Circles — chance nodes.
The bold outarcs from each decision node signify the optimal decision at that point.

Figure 9.1: Decision Tree

- The root is the starting state
- The leaves, commonly represented as triangles, are the outcomes and are labelled with the utility.
- Some of internal node are *decision nodes*, represented with squares. The outarcs from a decision node correspond to actions.
- The remaining internal nodes are *chance nodes*, represented with circles. The outarcs from a chance nodes correspond to events, and are labelled with the probability of the event.

The value of a decision node is the maximum of its children, and the prescribed action to take is the outarc that leads to the largest child. The value of a chance node is the expected value of its children. For a large tree, this is a more effective way of structuring the calculation than the enumeration of strategies above.

Figure 9.1 shows the decision tree for the restaurant problem. Decision trees are commonly drawn left to right, because a path from the root to a leaf moves forward in time. Figure 9.1 shows the *optimal strategy* highlighted with thicker arcs. The optimal strategy is obtained by deleting every suboptimal action and all its descendent nodes.

It should be noted that this is not the *complete* decision tree for this problem; that would also show obviously stupid actions, like going from one restaurant to another even if the first is quiet. In

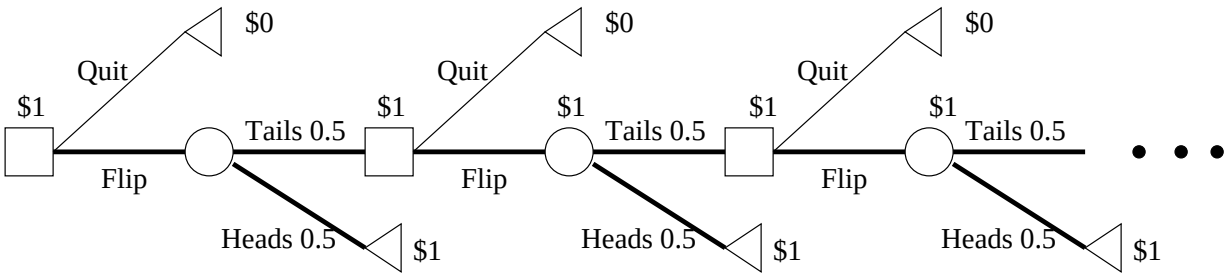


Figure 9.2: Infinite decision tree

fact, the complete decision tree is actually infinite, since the agent can go back and forth between restaurants arbitrarily many times. In this case, all but the actions shown in figure 9.1 are obviously suboptimal, and so need not be shown. (To be precise, for this probability model, these actions are easily to be seen to be outside the optimal strategy, whatever numeric values of the probabilities and waiting times are specified. Therefore, they can be excluded without doing any numerical calculations.)

In other problems, the tree of reasonable actions actually is infinite. For a simple example, suppose that someone makes you the following offer: You can flip a coin as many times as you want, and he will pay you $1 the first time it comes up heads. The expected value of this game is $1, since the probability is 1 that eventually some flip will come up heads. The decision tree for this case is shown in figure 9.2. Several kinds of data structures and algorithms have been developed that are more effective for these kinds of problem than decision trees, but they are beyond the scope of the discussion here.

To represent the probabilistic aspects of reasoning about complex strategies, we use a random variable "Outcome(A)" whose value is the utility of strategy A.[1] For instance let A be the plan, "Go to the Chinese restaurant and stay there even if it is busy"; let B be the event, "The Chinese restaurant is busy" and let F be the event, "Service is reasonably fast." Then we are given the following information.

$P(B) = 0.5$
$P(F|B) = 0.25$
Outcome(A)= { 20 if $\neg B$; 50 if $B \wedge F$; 80 if $B \wedge \neg F$ }.

Therefore,

$P(\text{Outcome}(A){=}20) = P(\neg B) = 0.5.$
$P(\text{Outcome}(A){=}50) = P(B, F) = P(F|B) \cdot P(B) = 0.125.$
$P(\text{Outcome}(A){=}80) = P(B, \neg F) = P(\neg F|B) \cdot P(B) = 0.375.$

So $\text{Exp}(\text{Outcome}(A)) = 0.5 \cdot 30 + 0.125 \cdot 50 + 0.375 \cdot 80 = 51.25$

9.3.2 Decision theory and the value of information

Decision theory also allows a value to be assigned to gaining information, in terms of the information's usefulness in helping to make decisions with better outcomes. For example, suppose that a book

[1] The problem of systematically representing strategies and calculating their various outcomes is the problem of *plan representation and reasoning;* it is beyond the scope of this book. See (Ghallab, Nau, and Traverso 2004) and (Russell and Norvig 2009).

manuscript has been submitted to a publisher. Let us make the following simplifying assumptions:

1. A book is either a success or a failure. If the book is a success, the publisher will gain $50,000. If the book is a failure, the publisher will lose $10,000.
2. The probability that a manuscript will succeed is 0.2 and the probability that it will fail is 0.8.

The publisher has a choice of two actions. He can publish the manuscript, in which case his expected gain is $0.2 * \$50,000 - 0.8 * \$10,000 = \$2000$. Or he can reject the manuscript, in which case his expected gain is $0. So his preferred plan is to publish the manuscript, for an expected gain of $2000.

Let us now suppose that the publisher has another option; namely, to consult with a reviewer. Consider, first, the case where the publisher knows an *infallible* reviewer, who can always successfully judge whether a book will succeed or fail. In that case, the publisher has the option of carrying out the following strategy:

Consult with the reviewer;
if (the reviewer recommends the book)
  then publish it;
  else reject it;

The expected value of this strategy can be calculated as follows. With probability 0.2 the book will be a success; the reviewer will approve it; the publisher will publish it, and will gain $50,000. With probability 0.8 the book will be a failure; the reviewer will reject it; the publisher will reject it, and will gain $0. Therefore the expected value of the outcome of this strategy, at the outset, is $0.2 \cdot \$50,000 + 0.8 \cdot 0 = \$10,000$. Therefore, the reviewer's opinion is worth $\$10,000 - \$2000 = \$8000$ to the publisher; if the reviewer's fee is less than $8000, then it is worthwhile to the publisher to pay it.

Unfortunately, reviewers are not actually infallible. The most that a publisher can realistically expect is that the reviewer's opinion bears some relation to the actual outcome. Let R be a Boolean random variable representing the reviewer's opinion; and let S be a random variable representing whether the book would be a success if the publisher publishes it. Suppose we are given the following additional conditional probabilities: $P(R = T \mid S = T) = 0.7$; and $P(R = T \mid S = F) = 0.4$.

Let $A1$ be the strategy discussed above: Publish if $R = T$, reject if $R = F$. Then we can evaluate $\text{Exp}(Outcome(S))$ as follows:

$$\text{Exp}(\text{Outcome}(A1)) =$$

$$\text{Exp}(\text{Outcome}(A1)|R = T) \cdot P(R = T) + \text{Exp}(\text{Outcome}(A1)|R = F) \cdot P(R = F)$$

If $R = F$ then the publisher does not publish; so $\text{Exp}(Outcome(A1)|R = F) = 0$. To evaluate the first term above we proceed as follows

$$\text{Exp}(\text{Outcome}(A)|R = T) \cdot P(R = T) =$$

$$\$50,000 \cdot P(S = T|R = T) \cdot P(R = T) - \$10,000 \cdot P(S = F|R = T) \cdot P(R = T) =$$

$$\$50,000 \cdot P(R = T|S = T) \cdot P(S = T) - \$10,000 \cdot P(R = T|S = F) \cdot P(S = F) =$$

$$\$50,000 \cdot 0.7 \cdot 0.2 - \$10,000 \cdot 0.4 \cdot 0.8 = \$3800$$

So $\text{Exp}(\text{Outcome}(A1)) = \$3800$. Thus the value of the reviewer's opinion is $\$3800 - \$2000 = \$1800$; as long as the reviewer charges less than $1800 it is worth consulting him.

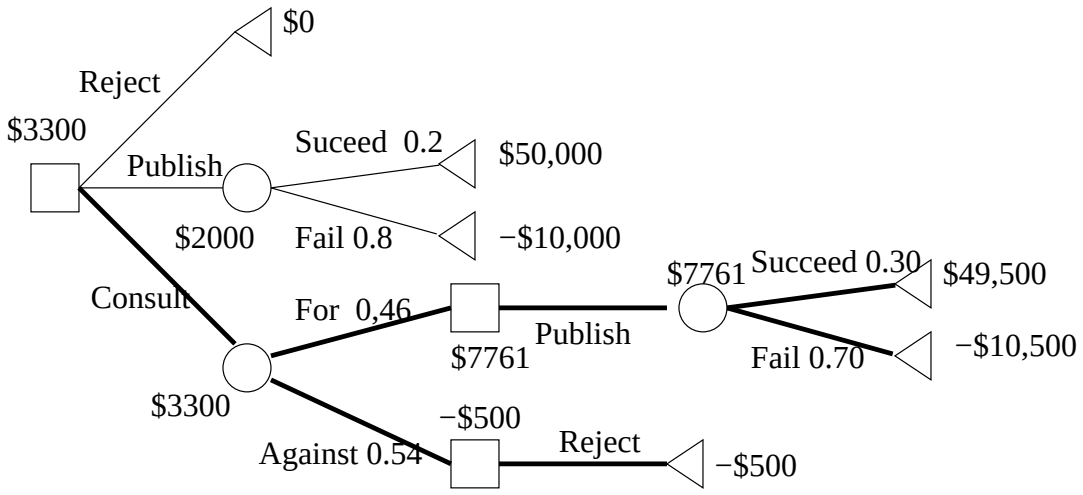


Figure 9.3: Decision tree for a publisher consulting with one reviewer

The decision tree for this problem is shown in figure 9.3. The reviewer's fee is taken to be $500. Again, obviously stupid choices of actions are omitted. For instance, there is no point in consulting unless the publisher is going to follow the reviewer's advice, so "reject" is not an option if a favorable review has been received, and "publish" is not an option if an unfavorable review has been received.

More complex versions of this problem, where the publisher has the option of hiring several reviewers, are considered in problems 9.2–9.3 and programming assignment 9.2.

As this kind of example gets more complex, the space of strategies becomes harder to characterize. (A small example of this is in exercise 9.3). Likewise the problem of determining whether a strategy is executable becomes more complex. Consider, for example, the following "strategy" $A2$: if $S = T$ then publish; else, reject. Clearly this is not actually a strategy. (The archetype of this kind of strategy is the advice, "Buy low, sell high.") But why is strategy $A1$ executable and $A2$ not executable? Or, more concretely, how does one develop a problem representation that will allow all and only executable strategies to be considered? Partial solutions are known, but the area is one of active research.

9.4 Variance and standard deviation

The expected value of X characterizes the center of the distribution X. The variance $\mathrm{Var}(X)$ and the standard deviation $\mathrm{Std}(X)$ characterize how broadly the distribution is spread around the center.[2]

Let X be a random variable and let v be a value. We will define the *spread* of X around v $\mathrm{Spread}(X, v)$ as the expected value of $(X - v)^2$. Note that this number $(X - v)^2$ is always positive and get larger the farther X is from v.

Clearly the most reasonable value of v to use to measure the inherent spread of X is the one that minimizes $\mathrm{Spread}(X, v)$. As luck would have it, that value of v is exactly $\mathrm{Exp}(X)$; and the associated value of the spread is called the *variance* of X, denoted $\mathrm{Var}(X)$.

As a measure of spread, however, the variance has the problem that it is in the wrong units; if X

[2]The expected value, variance, and standard deviation of a *random variable,* discussed in this chapter, should not be confused with the related concepts of the mean, variance, and standard deviation of a *data set,* discussed in chapter 14.

is measured in feet, for example, $\mathrm{Var}(X)$ is in square feet. To get a measure of the spread of X that is comparable to the values of X, we take the square root of the variance. This is the *standard deviation* of X, denoted $\mathrm{Std}(X)$.

Definition 9.1. *Let X be a numeric random variable. Let $\mu = \mathrm{Exp}(X)$. Then*

$$\mathrm{Var}(X) = \mathrm{Exp}((X-\mu)^2) = \sum_u P(X=u)(u-\mu)^2$$

$$\mathrm{Std}(X) = \sqrt{\mathrm{Var}(X)}$$

For example, let D be the roll of a single die. We calculated above that $\mathrm{Exp}(D) = 7/2$. Therefore:

$$\mathrm{Var}(D) =$$

$$(1/6)(1-7/2)^2+(1/6)(2-7/2)^2+(1/6)(3-7/2)^2+(1/6)(4-7/2)^2+(1/6)(5-7/2)^2+(1/6)(6-7/2)^2 =$$

$$1/6 \cdot (25/4 + 9/4 + 1/4 + 1/4 + 9/4 + 25/4) = 35/24 = 1.4583$$

$$\mathrm{Std}(D) = \sqrt{\mathrm{Var}(D)} = 1.2076$$

(You may ask, why use $\mathrm{Exp}((X-v)^2)$ rather than just $\mathrm{Exp}(|X-v|)$? That is also a useful number; the value of v that minimizes it is the *median* of X (see problem 9.4). But $(X-v)^2$ has a number of advantages. The simplest is that it is differentiable, which simplifies many symbolic manipulations such as minimization. Also, the variance satisfies the important theorem 9.6 below; there is no comparable theorem that holds for $\mathrm{Exp}(|X-v|)$.)

In probability theory, the symbol μ is often used for the expected value, and the symbol σ is used for the standard deviation, so σ^2 is the variance.

Clearly for any constant c, $\mathrm{Var}(X+c) = \mathrm{Var}(X)$, $\mathrm{Std}(X+c) = \mathrm{Std}(X)$, $\mathrm{Var}(c \cdot X) = c^2 \cdot \mathrm{Var}(X)$, and $\mathrm{Std}(c \cdot X) = c \cdot \mathrm{Std}(X)$. That is, the variance and standard deviation are invariant under translation and the standard deviation is linear under scalar multiplication.

The significance of the standard deviation is illustrated in the following theorem, known as Tschebyscheff's (also spelled Chebyshev, Čebisev, etc.) inequality:

Theorem 9.5. *Let X be a random variable with mean μ and standard deviation σ. Then for any $w > 0$, $P(|X-\mu| \geq w) \leq \sigma^2/w^2$. That is, if w is substantially greater than σ then it is very unlikely that X is more than w from μ, where "very unlikely" is σ^2/w^2.*

Proof: Let S be the set of all values of X, and let U be the subset of S of all values v of X such that $|v-\mu| \geq w$. Then for any value $u \in U$, $(u-\mu)^2 \geq w^2$ so $P(u) \cdot (u-\mu)^2 \geq P(u) \cdot w^2$. So

$$\sigma^2 = \sum_{v \in S} P(v) \cdot (v-\mu)^2 \geq \sum_{v \in U} P(v) \cdot (v-\mu)^2 \geq \sum_{v \in U} P(v) \cdot w^2 = w^2 \cdot \sum_{v \in U} P(v) = w^2 P(U)$$

So $P(|X-\mu| \geq w) = P(U) \leq \sigma^2/w^2$. ∎

The variance of the sum of two random variables, $\mathrm{Var}(X+Y)$ satisfies a theorem similar to theorem 9.3, *but it only applies if X and Y are independent:*

Theorem 9.6. *Let X and Y be* independent *random variables. Then* $\mathrm{Var}(X+Y) = \mathrm{Var}(X) + \mathrm{Var}(Y)$.

Proof: Let $\mu_X = \text{Exp}(X)$ and $\mu_Y = \text{Exp}(Y)$; these are constants. Let $\bar{X}$ and $\bar{Y}$ be the random variables $\bar{X} = X - \mu_X$, $\bar{Y} = Y - \mu_Y$. Then $\text{Exp}(\bar{X}) = \text{Exp}(X - \mu_X) = \text{Exp}(X) - \mu_X = 0$, and likewise $\text{Exp}(\bar{Y}) = 0$. Also $\bar{X} + \bar{Y} = X + Y - \mu_X - \mu_Y$ so $\text{Var}(\bar{X} + \bar{Y}) = \text{Var}(X + Y)$. By theorem 9.1, $\bar{X}$ and $\bar{Y}$ are independent.

So we have

$$
\begin{array}{l}
\text{Var}(X+Y) = \text{Var}(\bar{X}+\bar{Y}) = \\
\sum_{u,v}(u+v)^2 \cdot P(\bar{X}=u, \bar{Y}=v) = \\
\sum_{u,v}(u^2+2uv+v^2) \cdot P(\bar{X}=u, \bar{Y}=v) = \\
\sum_{u,v} u^2 \cdot P(\bar{X}=u, \bar{Y}=v) + \sum_{u,v} 2uv \cdot P(\bar{X}=u, \bar{Y}=v) + \sum_{u,v} v^2 \cdot P(\bar{X}=u, \bar{Y}=v) = \\
\sum_u u^2 \cdot [\sum_v P(\bar{X}=u, \bar{Y}=v)] + 2\,\text{Exp}(\bar{X} \cdot \bar{Y}) + \sum_v v^2 \cdot [\sum_u P(\bar{X}=u, \bar{Y}=v)] = \\
\sum_u u^2 \cdot P(\bar{X}=u) + 2\,\text{Exp}(\bar{X}) \cdot \text{Exp}(\bar{Y}) + \sum_v v^2 \cdot P(\bar{Y}=v) = \\
\text{Var}(\bar{X}) + \text{Var}(\bar{Y}) = \text{Var}(X) + \text{Var}(Y).
\end{array}
$$

In going from the fifth to the sixth line above, we used theorem 9.2 to add the marginal probabilities in the first and third term; and we used theorem 9.4 to convert $\text{Exp}(\bar{X} \cdot \bar{Y})$ to $\text{Exp}(\bar{X}) \cdot \text{Exp}(\bar{Y})$ since $\bar{X}$ and $\bar{Y}$ are independent. ∎

Using the above theorems we can derive the following important consequence:

Theorem 9.7. *Let $X_1 \ldots X_N$ be independent random variables, each with mean μ and standard deviation σ; thus $\text{Var}(X_i) = \sigma^2$. Let V be the average of these: $V = (X_1 + \ldots + X_N)/N$. Then*

a. $\text{Exp}(V) = (\text{Exp}(X_1) + \ldots + \text{Exp}(X_N))/N = \mu$.

b. $\text{Var}(V) = \text{Var}(X_1 + \ldots + X_N/N) = (\text{Var}(X_1) + \ldots + \text{Var}(X_N))/N^2 = \sigma^2/N$.

c. $\text{Std}(V) = \sqrt{\text{Var}(V)} = \sigma/\sqrt{N}$.

The key point is (c); the spread as measured by the standard deviation goes down proportional to the square root of the number of repetitions.

For example, suppose that we flip a coin 10,000 times. Let X_i be the random variable for the ith flip, with heads=1 and tails=0. Let V be the average of the X_i; thus V is the fraction of heads in the flips. We have $\text{Exp}(X_i) = 1/2$ and $\text{Std}(X_i) = 1/2$, so $\text{Exp}(V) = 1/2$ and $\text{Std}(V) = 1/200$. Using theorem 9.5 above, we can conclude that $P(|V - 1/2| \geq 1/100) \leq ((1/200)/(1/100))^2 = 1/4$. Thus there is at least a 0.75 chance that V is between 0.49 and 0.51. As we will see in section 9.8.2, this is a substantial underestimate — the true probability is 0.9545 — but we have been able to derive it with surprising ease.

9.5 Random variables over infinite sets of integers

(Note: This section requires an understanding of infinite sequences and infinite sums.)

The second category of numerical random variables are those whose domains is an infinite set of integers.

Example 9.3: Suppose that you repeatedly flip a coin until it turns up heads; then you stop. Let C be the random variable whose value is the number of flips you make. As in example 9.2, let $F_1, F_2 \ldots$ be random variables corresponding to the successive hits; the difference is that now we need an infinite sequence of random variables. Then

$P(C = 1) = P(F_1 = \text{H}) = 1/2.$
$P(C = 2) = P(F_1 = \text{T}, F_2 = \text{H}) = 1/4.$
$P(C = 3) = P(F_1 = \text{T}, F_2 = \text{T}, F_3 = \text{H}) = 1/8.$
...
$P(C = k) = 1/2^k.$
...

In general, we can let the sample space Ω be the set of natural numbers. A probability function over Ω is a function $P(i)$ such that $\sum_{i=1}^{\infty} P(i) = 1$. An event is a subset of Ω. The probability of event E, $P(E) = \sum_{x \in E} P(x)$. An unnormalized weight function $w(i)$ is any function such that the $\sum_{i=1}^{\infty} w(i)$ converges to a finite value.

Almost everything that we have done with finite random variables transfers over to this case, requiring only the change of finite sums to infinite sums. Otherwise, the definitions are all the same, the theorems are all the same, and the proofs are all the same, so we will not go through it all again. There are only three issues to watch out for.

First, axiom P.2 in the event-based axiomatization of probability has to be extended to infinite collections of events, as follows:

P.2′ Let $\{E_1, E_2, \ldots\}$ be a sequence of events, indexed by integers, such that, for all $i \neq j$, $E_i \cap E_j = \emptyset$. Then $P(E_1 \cup E_2 \cup \ldots) = P(E_1) + P(E_2) + \ldots$

The property described in this axiom is called *countable additivity*.

Second, there is no such thing as a uniform distribution over Ω. If all values in Ω have the same weight w, then, if $w > 0$ then the total weight would be infinite; if $w = 0$ then the total weight is zero. Neither of these is an acceptable alternative.

Third, a probability distribution may have an infinite mean; or a finite mean and an infinite variance. For example, the function distribution

$P(1) = 1/1 * 2 = 1/2.$
$P(2) = 1/2 * 3 = 1/6.$
$P(3) = 1/3 * 4 = 1/12.$
...
$P(k) = 1/k * (k + 1).$
...

is a legitimate probability distribution, since
$P(1) + P(2) + P(3) + \ldots + P(k) + \ldots = 1/1 * 2 + 1/2 * 3 + 1/3 * 4 + \ldots + 1/k(k + 1) + \ldots =$
$(1 - 1/2) + (1/2 - 1/3) + (1/3 - 1/4) + \ldots + (1/k - 1/k + 1) + \ldots = 1.$

However the expected value is $1 * P(1) + 2 * P(2) + 3 * P(3) + \ldots + k * P(k) + \ldots = 1/1 * 2 + 2/2 * 3 +$
$3/3 * 4 + \ldots + k/k(k + 1) + \ldots = 1/2 + 1/3 + 1/4 + \ldots + 1/(k + 1) + \ldots$, which is a divergent series.

Similarly, one can define a random variable X such that $P(X = k) = 1/k^2 - 1/(k+1)^2$ for $k = 1, 2, \ldots$. This is a legitimate probability distribution and has a finite mean, but the variance is infinite.

Therefore to extend any of the above theorems about $\text{Exp}(X)$ or $\text{Var}(X)$ to the case of random variables with infinite domains, one has to add the condition that $\text{Exp}(X)$ or $\text{Var}(X)$ exists and is finite.

9.6 Three important discrete distributions

In the theory of probability, mathematicians have studied many different specific distributions, with different kinds of applications and mathematical properties. These are generally families of distributions, each with a set of real- or integer-valued parameters; each assignment of values to the parameters gives a different distribution. In this book, we briefly discuss a few distributions that are particularly important in computer science applications. In this section we discuss three discrete distributions: the Bernoulli distribution, the binomial distribution, and the Zipf distribution. Continuous distributions will be discussed in section 9.8.

9.6.1 The Bernoulli distribution

The Bernoulli distribution is associated with a single flip of a weighted coin. It has one parameter p, the probability that the flip comes up heads. The domain is the set $\{0, 1\}$. The distribution is defined as follows:

$P(X = 1) = p.$
$P(X = 0) = (1 - p).$

The expectation $\text{Exp}(X) = p$. The variance $\text{Var}(X) = p(1-p)$. The Bernoulli distribution is a very simple one in itself, but it is a basic component of more complex distributions.

9.6.2 The binomial distribution

Suppose that you have a weighted coin, which comes up heads with probability p, and you flip it n times. Let X be the random variable whose value is the number times the coin comes up heads in the n flips. Then the probability distribution for X is the *binomial distribution*.

The binomial distribution has two parameters: n and p. It takes on values in $\{0, 1, \ldots n\}$. We can calculate $P(X = k)$ as follows: Any particular sequence of with k heads and $n - k$ tails has probability $p^k \cdot (1 - p)^{n-k}$. For example, if $p = 0.75$, $k = 2$, $n = 5$ then the probability of the particular sequence HTTHT is

$$p \cdot (1 - p) \cdot (1 - p) \cdot p \cdot (1 - p) = p^2 \cdot (1 - p)^3 = 0.0088$$

Any sequence of k heads and $n - k$ tails corresponds to one way of choosing the k positions for the heads out of the n positions in the sequence; the number of such sequences is therefore $C(n, k) = n!/k! \cdot (n - k)!$ For example, the number of sequences with 2 heads and 3 tails is $5!/2! \cdot 3! = 10$. The total probability of getting k heads in a sequence of n flips is therefore

$$P(X = k) = B_{n,p}(k) = C(n, k) \cdot p^k \cdot (1 - p)^{n-k} = \frac{n!}{k!(n - k)!} \cdot p^k \cdot (1 - p)^{n-k}$$

For example, for $n = 5, p = 3/4$, the distribution is

$P(X = 0) = 5!/(5! \cdot 0!) \cdot (3/4)^0(1/4)^5 = 1 \cdot 1/4^5 = 0.0098$
$P(X = 1) = 5!/(4! \cdot 1!) \cdot (3/4)^1(1/4)^4 = 5 \cdot 3^1/4^5 = 0.0146$
$P(X = 2) = 5!/(3! \cdot 2!) \cdot (3/4)^2(1/4)^3 = 10 \cdot 3^2/4^5 = 0.0878$
$P(X = 3) = 5!/(2! \cdot 3!) \cdot (3/4)^3(1/4)^2 = 10 \cdot 3^3/4^5 = 0.2636$
$P(X = 4) = 5!/(1! \cdot 4!) \cdot (3/4)^4(1/4)^1 = 5 \cdot 3^4/4^5 = 0.3955$
$P(X = 5) = 5!/(0! \cdot 5!) \cdot (3/4)^5(1/4)^0 = 1 \cdot 3^5/4^5 = 0.2373$

the	6,187,267	in	1,812,609	was	923,948	you	695,498	on	647,344
of	2,941,444	to	1,620,850	to	917,579	he	681,255	that	628,999
and	2,682,863	it	1,089,186	I	884,599	be	662,516	by	507,317
a	2,126,369	is	998,389	for	833,360	with	652,027	at	478,162

Table 9.2: Frequencies of the 20 most common words

1	486,507	5	25,065	9	9,765	13	5,534	17	3,588
2	123,633	6	19,109	10	8,551	14	5,079	18	3,389
3	58,821	7	14,813	11	7,419	15	4,506	19	3,089
4	36,289	8	11,905	12	5,817	16	4,016	20	2,856

Table 9.3: Number of words that occur rarely

The random variable X is the sum of n independent random variables B_i each with the Bernoulli distribution. Therefore, by theorems 9.3 and 9.6,

$$\mathrm{Exp}(X) = \mathrm{Exp}(B_1) + \ldots + \mathrm{Exp}(B_n) = n * \mathrm{Exp}(B_1) = np.$$
$$\mathrm{Var}(X) = \mathrm{Var}(B_1) + \ldots + \mathrm{Var}(B_n) = n * \mathrm{Var}(B_1) = np(1-p).$$

9.6.3 The Zipf distribution

Take a large corpus of English text, count the frequency of every word, and list them in decreasing order. For example, the British National Corpus is a collection of representative English texts. It is 100,106,029 words long and contains 938,972 different words. (An occurrence of a word is called a "token"; different words are called "types".) Table 9.2 shows the number of occurrences of the 20 most common words in the corpus.[3]

Let us consider the number of occurrences as a function of the rank of the word; that is, $f(1) = 6,187,267$, $f(2) = 2,941,444$ and so on. It turns out that the function

$$y(n) = 13,965,000 * (n + 0.8948)^{-1.0854}$$

fits this data very well. This can be seen by using a log-log plot where $x = n + 0.8948$; the curve becomes the straight line $\log(y) = -1.0854 \log(x) + \log(13,965,000)$. Figure 9.4 shows the first 200 data points and the line; as can be seen, the agreement is very close except for the value $n = 2$.

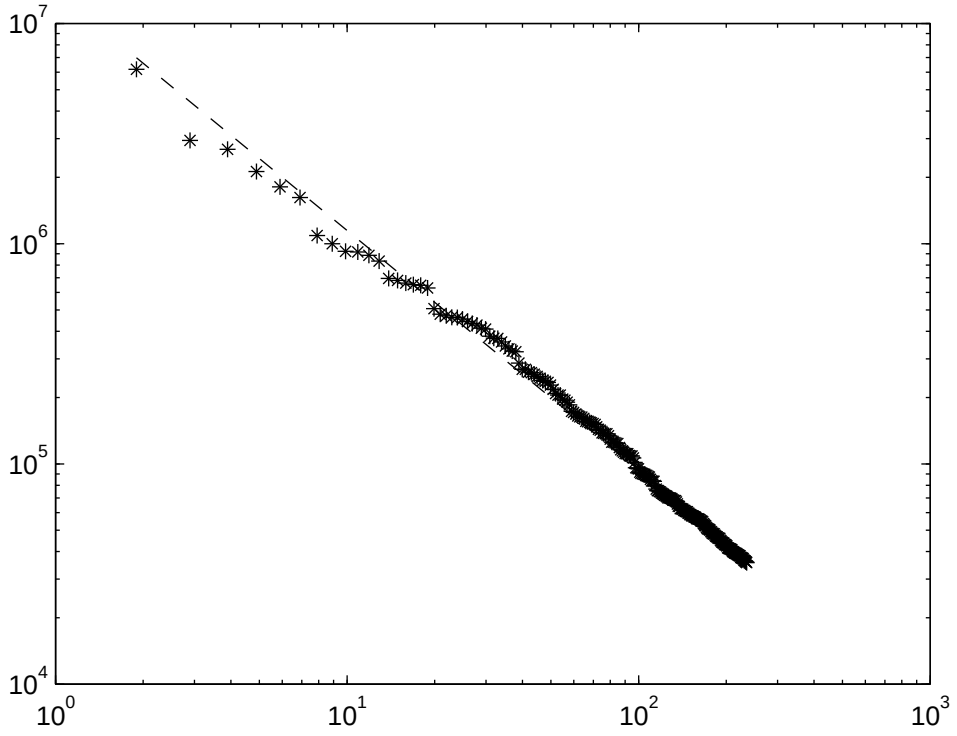
This can be turned into a probability distribution by normalization; the probability of word w is the number of its occurrences in the corpus divided by the length of the corpus.

At the other end of frequency, let us consider the most uncommon words in the corpus, and count the number of words that occur a very small number of times. In this corpus, there are 486,507 words that occur once; 123,633 words that occur twice, and so on (Not all of these are words in the usual sense; this count includes numerals and some other non-word textual elements.) Table 9.3 shows the data up to words that occur 20 times.

This data fits very well to the curve $f(n) = 399,000 \cdot n^{-1.669}$. If we plot the data on a log-log scale, the fit to a straight line appears so perfect that it is not worth drawing the line.

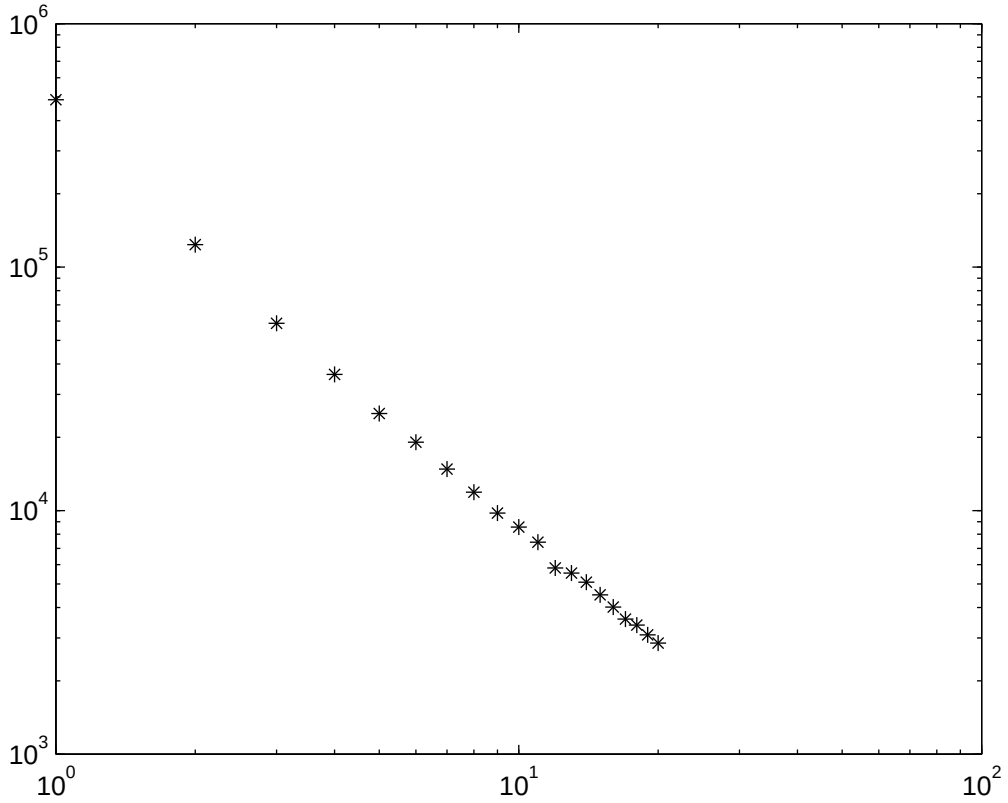
Distributions of the form $\alpha(n+\beta)^{-\gamma}$ are called *Zipf* distributions, or *inverse power law*, or *long tail* or

[3] "BNC database and word frequency lists" by Adam Kilgarriff, http://www.kilgarriff.co.uk/bnc-readme.html, 8/30/10. The data separates occurrences of words by part of speech; thus the first "to" in the table is as a particle and the second is as a preposition. The figure for "that" is as a conjunction.



The data is shown in red asterisk. The blue solid line is the best fit.

Figure 9.4: Occurrences of 200 common words by rank: log-log plot



The data points are marked with red asterisks.

Figure 9.5: Number of words with very low frequency

fat tail distribution.[4] Many diverse phenomena follow a Zipf distribution, including: word frequency; city population; company size; number of pages published by scientists; magazine circulation; movie popularity; number of accesses to web pages; number of inlinks to web pages; number of outlinks from web pages; size of strongly connected components in the web; personal wealth and personal income; and many others.[5]

A number of important features of the Zipf distribution should be noted. We will describe these and illustrate them using our first example of word distribution, but they apply generally.

First, the top elements account for a substantial proportion of the total. In the word frequency example, the 10 most common words comprise 21% of all the token; the 20 most common words comprise 28% of all tokens. The top 175 words comprise 50% of all tokens.

Second, infrequent elements also, collectively, account for a substantial proportion of the total. In the word frequency example, words that appear only once comprise 0.5% of the total. Words that appear at most ten times comprise 1.7% of the total. Words that appear at most twenty times comprise 2.3% of the total. This is the *long tail* or *fat tail* effect; the probability that a random token in a corpus is a very low-ranked word is much greater than with other common distributions.

To underline the force of this, let us compare what would happen if the words were evenly distributed; that is, if each token had equal probability of being any of the 938,000 types. Let $n \approx 10^8$ be the total length of the corpus; and let $p \approx 10^{-6}$ be the frequency of each word. For each word w let X_w be the random variable whose value is the number of occurrences of w in the corpus; then X follows the binomial distribution $P(X = k) = B_{n,p}(k)$. Using an asymptotic analysis one can show (these are order of order of magnitude calculations; that is, the exponent is within a factor of 2 or so);

- $P(X = 1) \approx 10^2 e^{-100} \approx 10^{-41}$. Therefore the probability that the corpus would contain any word that occurs only once is about 10^{-35}. The probability that the corpus would contain 500,000 such words is about $10^{-1.7 \cdot 10^7}$.
- $P(X \geq 6 \cdot 10^6) \approx 10^{-2.4 \cdot 10^7}$ Therefore the probability that the corpus contains any word occurring six million or more times in the corpus is likewise about $10^{-2.4 \cdot 10^7}$.

Small values of the exponent γ favor the second effect — the tail is long — large values of γ favor the first effect — the large elements are very large.

Third, power law distributions tend to give rise to computational problems where it is easy to make great strides at the start and then progressively harder to make improvements. For example consider the probability p_q that, after reading the first q words of the corpus, the next word that you read is one that you have seen already. If the words follow a power law with exponent approximately -1, one can show that, for a wide range of C, p_q increases *logarithmically* as a function of q, and thus the C required to achieve a given value of p_C increases exponentially as a function of p.

Table 9.4 illustrates how this probability increases with the number of words read, in the case of a total vocabulary of $100,000$ different words and a distribution proportional to $1/k$. Note that at each stage, doubling the number of words you have read increases the probability by about 5.5%. In this table q is the number of words that have been read. The value p is the probability that the next word you read will be one that you have seen, as given by a Monte Carlo simulation; these numbers are accurate to within the two digits given here. (See exercise 12.6 for the programming of this simulation.). The value $\tilde{p}$ is the value estimated by the approximate theoretical computation at the end of this section.

[4] This is sometimes called "Zipf's law", but the only "law" is that many things follow the distribution.

[5] S. Sinha and R.K. Pan, "How a "Hit" is Born: The Emergence of Popularity from the Dynamics of Collective Choice." in B.K. Chakarabarti, A. Chakraborti, and A. Chatterjee, (eds.) *Econophysics and Sociophysics: Trends and Perspectives,* Berlin:Wiley 2006. It is debated whether some of these may actually be very similar distributions, such as log-normal distribution; but for our purposes here it hardly matters.

q	p	$\tilde{p}$	q	p	$\tilde{p}$	q	p	$\tilde{p}$	q	p	$\tilde{p}$
100	0.28	0.21	200	0.33	0.27	400	0.39	0.32	800	0.44	0.38
1600	0.50	0.44	3200	0.56	0.49	6,400	0.61	0.55	12,800	0.66	0.61
25,600	0.73	0.67	51,200	0.78	0.72	102,400	0.84	0.78	204,800	0.89	0.84

Table 9.4: Probability that you have seen the next word

The consequence of this is a phenomenon often encountered in artificial intelligence research; you can easily get results that seem promising, and with a reasonable amount of work you can get results that are fairly good, but getting really good results requires a lot more work, and excellent results seem to be entirely out of reach.

For actual individual words, as above, these results don't actually matter so much, for two reasons. First, a corpus of 1,000,000 words or even 100,000,000 words is actually reasonably easy to collect, and to do basic forms of analysis on, so it's not that daunting. Second, individual words are largely arbitrary; broadly speaking, words have to be learned one at a time, so there is no way to learn the properties of a word until you have seen it. If you want to collect a lexicon with 500,000 different words, you will have to work through a corpus that contains 500,000 different words; there is no choice. By contrast, if you have an application that requires knowing the properties of 1 billion different 3-grams (triples of consecutive words — see section 10.3), it may not be necessary to examine a text corpus that contains 1 billion different 3-grams, because 3-grams are not arbitrary; there is a logic to the possible or probable sequences of words.

Power law distributions with small exponents have anomalous behavior as regards the mean and the variance. A distribution $p_n = \alpha n^{-\gamma}$ has an infinite variance if $\gamma \leq 3$; it has an infinite mean if $\gamma \leq 2$; and it is not a probability distribution at all if $\gamma \leq 1$ because the sum $\sum 1/n^\gamma$ diverges for $\gamma \leq 1$. In this last case, one must assume that there are only a finite number of values, as we have done in computing table 9.4. If γ is just above the critical values 3 or 2, then the variance and the mean are anomalously large. Therefore if you are computing mean and variance from statistical values and one or both seem strangely large and very unstable from one sample to another, then you should suspect that you may be dealing with a power law distribution, and that computations based on mean and variance may not be meaningful.

Deriving the probability that you have seen the next word

Let H_k be the harmonic sum $H_k = \sum_{i=1}^{k}(1/i)$. Then it is known that $H_k = \ln(k) + \gamma + O(1/k)$ where $\gamma \approx 0.5772$ is known as Euler's constant.

Let W be the size of the vocabulary. Let w_k be the kth ranked word, for $k = 1 \ldots W$. Assume that the frequency of w_k in text is proportional to $1/k$. Then the normalization factor is H_W, so the probability that a random token is w_k is $p_k = 1/(k \cdot H_W)$.

Suppose that you have read a random text T of q tokens, where $H_W \ll q \ll WH_W$. Suppose that last token you read was a word you have seen before; then it is one of those words that occurs at least twice in the text. Since "being the last word in the text" is independent of "occurring at least twice in the text", the probability that the last word you read was one you had already seen is equal to the fraction of tokens in T whose word occur at least twice in T. We can roughly assume that the text contains at least two occurrences of word w_k if $qp_k > 3/2$; this holds if $k \leq 2q/3H_W$. Let $r = 2q/3H_W$. Then the fraction of tokens in T whose word occurs at least twice in T is $H_r/H_W = \ln(3q/2H_W)/H_W$.

Table 9.4 shows the estimate $\bar{p}$ derived from this argument and the much more accurate estimate p

derived from Monte Carlo simulation, for various values of n. Over the entire range of n, $\bar{p} \approx p - 0.05$ thus plotting p against $\log(n)$, the argument gets the y-intercept wrong by about 0.05, but gets the slope almost exactly correct.

9.7 Continuous random variables

(Note: This section requires calculus, and at one critical point it requires multivariable calculus.)

The third category of numerical random variable are random variables that take values over the real line. The theory here is different and more difficult than with finite domains or integer domains.

The sample space Ω is the real line $\mathbb{R}$. However, unlike the sample spaces we have looked at earlier, the probability of an event is not derived from the probabilities of individual elements; typically, each individual element has probability zero. Rather the probability of events is a characteristic of the interval as a whole, just as the length of an interval is not the sum of the lengths of the points in the interval.

Specifically: We posit that there is a large[6] collection of subsets of $\mathbb{R}$ called the *measurable* sets. If X is a random variable with domain $\mathbb{R}$ and E is a measurable set, then $X \in E$ is a probabilistic event, and $P(X \in E)$ is a probabilistic event satisfying axioms P.1, P.2′, P.3, and P.4.

Notice that this is something like what we did in the likelihood interpretation of probability, in the sense that we took the probability of events as a starting point. However, in that earlier analysis, we were able to form a finite sample space of elements by combining events; here that is not possible.

From the above description it sounds as though, in order to specify a probability distribution, we would have to specify $P(X \in E)$ separately for all measurable E, which would be a large undertaking. Fortunately, because of the axioms constraining probability distributions, there is a simpler approach: the probability of all events can be specified by specifying the *cumulative distribution*.

Definition 9.2. *Let $c(t)$ be a continuous function from $\mathbb{R}$ into the closed interval [0,1] such that*

- *$c(t)$ is monotonically non-decreasing; that is, if $t_1 \leq t_2$ then $c(t_1) \leq c(t_2)$.*
- *For any v such that $0 < v < 1$, there exists t such that $c(t) = v$.*

Let X be a numeric random variable. Then c is the cumulative distribution function (c.d.f.) *for X if, for every t, $P(X \leq t) = P(X < t) = c(t)$.*

(One can give a more general definition that allows c to be discontinuous from the left, and weakens some of the other conditions; however, we will not need that level of generality here.)

If we have specified a cumulative distribution $c(t)$ for a random variable X, then that determines the probability that X lies within any specified interval $[u, v]$:

$$P(X \in [u, v]) = P(X \leq v \wedge \neg(X < u)) = P(X \leq v) - P(X < u) = c(v) - c(u)$$

We can then use axiom P.2′ to calculate $P(X \in E)$ where E is the union of a finite set of intervals or of an infinite set of intervals

Example 9.4: Let $c(t)$ be the following function (Figure 9.7)

[6] The question of *what* subsets of $\mathbb{R}$ can be considered measurable is a very deep one. However, certainly any finite union of intervals is measurable, which is all that we will need.

for $t < 0$, $c(t) = 0$.
for $0 \le t \le 1$, $c(t) = t$.
for $t > 1$, $c(t) = 1$.

Clearly $c(t)$ satisfies the conditions of definition 9.2. Let X be a random variable X with distribution $c(t)$. For that distribution we have

$$P(X \in [u,v]) = c(v) - c(u) = \begin{cases} \text{if } u \le v \le 0 \text{ then } 0 \\ \text{if } u \le 0 \text{ and } 0 \le v \le 1 \text{ then } v \\ \text{if } 0 \le u \le v \le 1 \text{ then } v - u \\ \text{if } 0 \le u \le 1 \text{ and } 1 \le v \text{ then } 1 - u \\ \text{if } 1 \le u \le v \text{ then } 0 \end{cases}$$

If E is the union of disjoint intervals, then $P(E)$ is the sum of their probabilities. For example $P(X \in [-1, 1/6] \cup [1/3, 2/3] \cup [5/6, 2]) = 1/6 + 1/3 + 1/6 = 2/3$.

A more useful, though slightly less general, way to represent continuous distribution is in terms of the *probability density.*

Definition 9.3. *Let X be a random variable with cumulative distribution $c(t)$. If $c(t)$ is piecewise differentiable (i.e. differentiable at all but isolated points) then the derivative of c, $f(t) = c'(t)$ is the* probability density *associated with X. (The value of f at the points where c is not differentiable does not matter.)*

Another, more direct definition of f is as follows: For any point t,

$$f(t) = \lim_{u \to t, \epsilon \to 0^+} \frac{P(u < X < u + \epsilon)}{\epsilon}$$

So $f(t)$ is the probability that X lies in a interval of length ϵ near t, divided by the length ϵ. (If this does not approach a unique limit, then the value of $f(t)$ is arbitrary and may be assigned arbitrarily. For reasonable probability distributions, this will only happen at isolated points.)

A density function is essentially the limit of a series of histograms, with the subdivision on the x-axis gets smaller and smaller. At each stage, the y-axis is rescaled to be inversely proportional to the division, so that the height of each rectangle remains roughly constant.

For example, consider the density function $\tilde{P}(X = t) = (3/4)(1-t^2), -1 \le t \le 1$. The corresponding cumulative function is the integral

$$c(t) = \int_{-1}^{t} \frac{3}{4}(1 - x^2)dx = -\frac{1}{4}t^3 + \frac{3}{4}t + \frac{1}{2}$$

Thus

$$P(t - \Delta \le X \le t + \Delta) = c(t + \Delta) - c(t - \Delta) = -\frac{3t^2\Delta}{2} - \frac{\Delta^3}{2} + \frac{3\Delta}{2}$$

Rescaling by the width 2Δ, we have

$$\frac{P(t - \Delta \le X \le t + \Delta)}{2\Delta} = \frac{3 - 3t^2 - \Delta^2}{4}$$

Note that as Δ goes to zero, this converges to the density $(3/4)(1 - t^2)$. Figure 9.6 shows a series of bar charts for $P(t - \Delta \le X \le t + \Delta)/2\Delta$ for $\Delta = 1/4, 1/8, 1/16$, and the density function with $-1 \le t \le 1$.

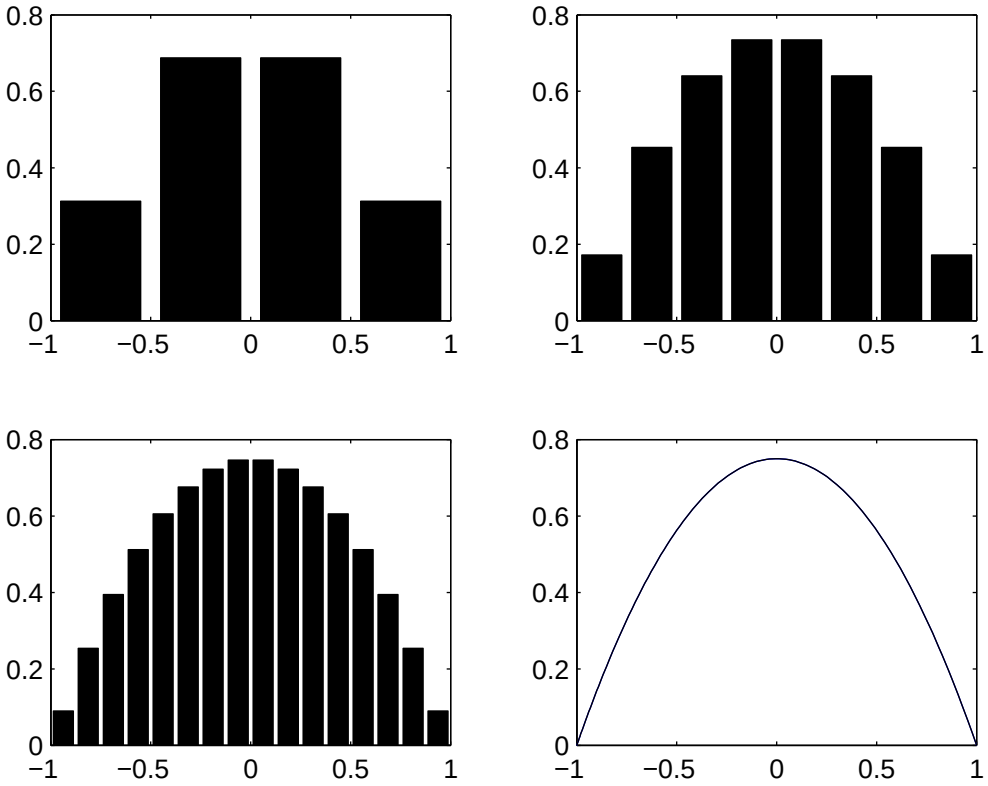


Figure 9.6: Probability density as a limit of histograms

We will write $\tilde{P}(X = t)$ for the value at t of the probability density of X. (This is a slight abuse of notation, but should not cause confusion.) Thus we have

$$\tilde{P}(X = t) = \frac{d}{dt}P(X \leq t)$$

The probability $P(X \in E)$ is the integral of the p.d.f. of X over E.

Theorem 9.8. *Let X be a random variable over $\mathbb{R}$ and let E be a measurable subset of $\mathbb{R}$. Then*

$$P(X \in E) = \int_{t \in E} \tilde{P}(X = t)dt$$

Example 9.4, continued: The random variable defined in example 9.4 above has the probability density $f(t)$ where

For $t < 0$, $f(t) = 0$.
For $0 \leq t \leq 1$, $f(t) = 1$.
For $t > 1$, $f(t) = 0$.

Since the cumulative function $c(t)$ is not differentiable at $t = 0$ and $t = 1$, the values of f at those points is not defined, and may be chosen arbitrarily.

Example 9.5: Let X be a random variable with cumulative distribution $c(t) = e^t/(1 + e^t)$. Since e^t goes from 0 to ∞ as t goes from $-\infty$ to ∞, and e^t is a continuous increasing function, it is easily checked that $c(t)$ satisfies the conditions of definition 9.2. Then the p.d.f. of X, $\tilde{P}(X = t) = dc/dt = e^t/(1 + e^t)^2$ (Figure 9.8).

In many ways, the probability density function $f(t)$ over elements $t \in \mathbb{R}$ looks a lot like a probability function over a finite sample space Ω, where summation in the finite case is replaced by integration in the continuous case, and we will discuss many of those parallels below. Before we do that, however, let us emphasize that they are *not* the same thing, and that there are important differences. One difference is that a probability density function may be greater than 1, as long as the integral is 1. Example 9.6 illustrates this.

Example 9.6: The following function is a legitimate probability density function:

For $t < 0$, $h(t) = 0$.
For $0 \leq t \leq 1/2$, $h(t) = 2$.
For $t > 1/2$, $h(t) = 0$.

Second, probability densities behave differently from probabilities on elements as regards functions of a random variable. If X is a random variable, and g is an injection (invertible function), then for any value v, $P(g(X) = g(v)) = P(X = v)$. But it is not the case for probability densities that $\tilde{P}(g(X) = g(v)) = \tilde{P}(X = v)$ because g changes not only the value of v but also the scale in the neighborhood of t. For instance, let X be the random variable of example 9.4. Let $g(v) = v/2$. Then the random variable $g(X)$ has the density $h(t)$ discussed above in example 9.6; thus $\tilde{P}(g(X) = g(t)) = 2 \cdot \tilde{P}(X = t)$. The explanation is as follows. Let t be any value such that $0 < t < 1/2$ and let ϵ be small. Then

$$\tilde{P}(g(X) = g(t)) \approx \frac{1}{\epsilon} \cdot P(g(t) \leq g(X) \leq g(t) + \epsilon) = \frac{1}{\epsilon} \cdot P(\frac{t}{2} \leq \frac{X}{2} \leq \frac{t}{2} + \epsilon) =$$

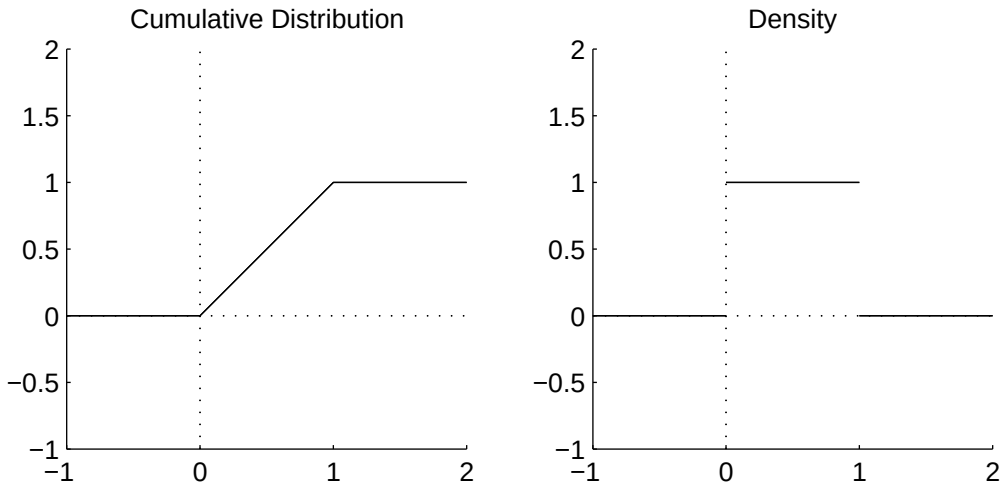
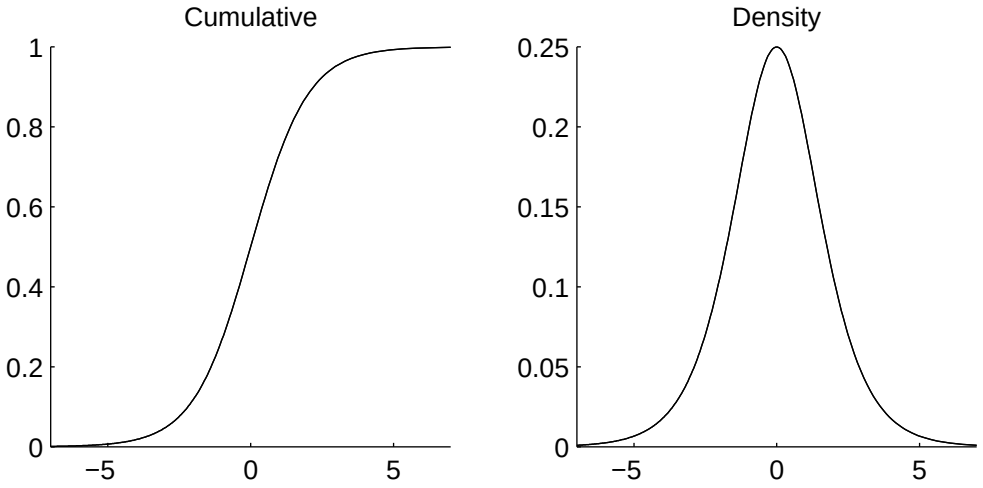


Figure 9.7: Example 9.4



Cumulative distribution: $e^t/(1+e^t)$. Density: $e^t/(1+e^t)^2$.

Figure 9.8: Example 9.5

$$\frac{1}{\epsilon} \cdot P(t \leq X \leq t + 2\epsilon) = 2 \cdot \frac{1}{2\epsilon} \cdot P(t \leq X \leq t + 2\epsilon) \approx 2 \cdot \tilde{P}(X = t)$$

An alternative derivation (essentially equivalent, but perhaps easier). Let $c(t)$ be the cumulative distribution function defined in example 9.4:

for $t < 0$, $c(t) = 0$.
for $0 \leq t \leq 1$, $c(t) = t$.
for $t > 1$, $c(t) = 1$.

Let X be a random variable whose c.d.f. is $c(t)$; that is $P(X \leq t) = c(t)$ Then

$$\tilde{P}(X = t) = \frac{d}{dt} P(X \leq t) = \frac{d}{dt} c(t) = h(t)$$

Let $Y = G(X)$. Then

$$\tilde{P}(Y = u) = \frac{d}{du} P(Y \leq u) = \frac{d}{du} P(X \leq 2u) = \frac{d}{du} c(2u) = 2h(2u) = 2\tilde{P}(X = 2u)$$

So if $t = 2u$ then $\tilde{P}(Y = u) = \tilde{P}(G(X) = G(t)) = 2\tilde{P}(X = t)$.

Generalizing the above calculation, one can show that, for any differentiable invertible function $G(v)$, if X has density $f(t)$ then $G(X)$ has density $f(G(t))/G'(t)$.

In many ways, however, p.d.f.'s do work in the same way as probability functions, replacing summation by integration. Let X be a discrete numeric random variable with probability function $P(x)$ and let Y be a continuous random variable with p.d.f. $\tilde{P}(t)$. Then

Probability Functions	Density functions
for all $v, P(v) \geq 0$	for all $v, \tilde{P}(v) \geq 0$
$1 = \sum_v P(v)$	$1 = \int_{-\infty}^{\infty} \tilde{P}(v)dv$
$\text{Exp}(X) = \sum_v v \cdot P(v)$	$\text{Exp}(Y) = \int_{-\infty}^{\infty} v \cdot \tilde{P}(v)dv$
$\text{Var}(X) = \sum_v (v - \text{Exp}(X))^2 \cdot P(v)$	$\text{Var}(Y) = \int_{-\infty}^{\infty} (v - \text{Exp}(Y))^2 \cdot \tilde{P}(v)dv$

Moreover, as with discrete probabilities, it is often convenient to use an unnormalized weight function $w(v)$. A function $w(v)$ can serve as a weight function if it satisfies the conditions that $w(v) \geq 0$ for all v, and that $\int_{-\infty}^{\infty} w(v)dv$ is finite but greater than 0. The p.d.f. associated with weight function $w(v)$ is $f(v) = w(v)/\int_{-\infty}^{\infty} w(v)dv$.

The theorems that combine several random variables also carry over to the continuous case; however, to make them meaningful, we need to define the meaning of a joint probability distribution and of a joint density function. (It is possible to define a joint cumulative distribution function, but it is awkward and not very useful.)

We posit that there exists a collection of measurable subsets of $\mathbb{R}^n$. A probability function over the measurable subsets of $\mathbb{R}^n$ is a function $P(E)$ mapping a measurable set E to a value in [0,1] satisfying axioms P.1, P.2′, P.3, and P.4.

Definition 9.4. *Let $\langle X_1, X_2 \ldots X_n \rangle$ be a finite sequence of continuous random variables. Then the* joint distribution of $\langle X_1 \ldots X_n \rangle$*, denoted $P(\langle X_1 \ldots X_n \rangle \in E)$, is a probability function over the measurable sets E.*

Definition 9.5. *Let $\langle X_1, X_2 \ldots X_n\rangle$ be a finite sequence of continuous random variables and let $P(\langle X_1 \ldots X_n\rangle \in E)$ be its probability function. Let $\vec{t} = \langle t_1 \ldots t_n\rangle$ be a vector in $\mathbb{R}^n$. The probability density function of $\langle X_1, X_2 \ldots X_n\rangle$ satisfies the following: For any $\vec{t}$*

$$\tilde{P}(X_1 = t_1 \ldots X_n = t_n) = \lim_{\vec{u}\to\vec{t},\epsilon\to 0^+} \frac{P(u_1 \le X_1 \le u_1 + \epsilon \wedge \ldots \wedge u_n \le X_n \le u_n + \epsilon)}{\epsilon^n}$$

if that limit exists.

That is, the probability density at $\vec{t}$ is the probability that $\langle X_1 \ldots X_n\rangle$ lies in an n-dimensional box of side ϵ near t, divided by the volume of the box, ϵ^n.

If there is no unique limit at a point $\vec{t}$ then the value of $f(\vec{t})$ does not matter. If P is a "well-behaved" function then the set of points where the limit does not exist has measure zero.

As in the one-dimensional case the probability can be gotten from the density by integrating:

Theorem 9.9. *Let $X_1, X_2 \ldots X_n$ be continuous random variables and let E be a measurable subset of $\mathbb{R}^n$. Then*

$$P(\langle X_1 \ldots X_n\rangle \in E) = \int \ldots \int_E \tilde{P}(X_1 = t_1 \ldots X_n = t_n) dt_1 \ldots dt_n$$

Virtually all of the theorems we have proven for discrete probabilities now carry over to continuous probabilities, replacing summation by integration. For simplicity, we will state them in terms of two random variables, but they all generalize in an obvious way to n random variables. In all of the following, X and Y are continuous random variables.

Theorem 9.10. *X is independent of Y if and only if for all values t and u, $\tilde{P}(X = t, Y = u) = \tilde{P}(X = t) \cdot \tilde{P}(Y = u)$.*

The conditional density distribution is defined as $\tilde{P}(X = t \mid Y = v) = \tilde{P}(X = u, Y = v)/\tilde{P}(Y = v)$

The following is the basic theorem about marginal probabilities, analogous to theorem 9.2.

Theorem 9.11. *For any value t of X,*

$$\tilde{P}(X = t) = \int_{-\infty}^{\infty} \tilde{P}(X = t, Y = u) du$$

Theorem 9.12. *Let v be a particular value of Y such that $\tilde{P}(Y = v) \neq 0$. Then the conditional density $\tilde{P}(X = u \mid Y = v) = \tilde{P}(X = u, Y = v)/\tilde{P}(Y = v)$ is a probability density as a function of u.*

The wording of theorems 9.3-9.7 is exactly the same in the continuous case as in the discrete infinite case. The proofs are exactly the same as in the finite case, replacing sums by integrals.

Theorem 9.3: If $\mathrm{Exp}(X)$ and $\mathrm{Exp}(Y)$ are finite then $\mathrm{Exp}(X + Y) = \mathrm{Exp}(X) + \mathrm{Exp}(Y)$.

Theorem 9.4: If $\mathrm{Exp}(X)$ and $\mathrm{Exp}(Y)$ are finite and X and Y are independent, then $\mathrm{Exp}(X \cdot Y) = \mathrm{Exp}(X) \cdot \mathrm{Exp}(Y)$.

Theorem 9.5: Let X be a random variable with mean μ and standard deviation σ. Then for any $w > 0$, $P(|X - \mu| \ge w) \le \sigma^2/w^2$.

Theorem 9.6: If $\mathrm{Var}(X)$ and $\mathrm{Var}(Y)$ are finite and X and Y are independent, then $\mathrm{Var}(X + Y) = \mathrm{Var}(X) + \mathrm{Var}(Y)$.

Theorem 9.7: Let $X_1 \ldots X_N$ be independent random variables, each with mean μ and standard deviation σ; thus $\mathrm{Var}(X_i) = \sigma^2$. Let V be the average of these: $V = (X_1 + \ldots + X_N)/N$. Then

a. $\text{Exp}(V) = (\text{Exp}(X_1) + \ldots + \text{Exp}(X_N))/N = \mu$.

b. $\text{Var}(V) = \text{Var}(X_1 + \ldots + X_N/N) = (\text{Var}(X_1) + \ldots + \text{Var}(X_N))/N^2 = \sigma^2/N$.

c. $\text{Std}(V) = \sqrt{\text{Var}(V)} = \sigma/\sqrt{N}$.

9.8 Two important continuous distributions

9.8.1 The continuous uniform distribution

The uniform distribution is a generalization of examples 9.4 and 9.6. The uniform distribution has two parameters: a lower bound L and upper bound U where $L < U$; it has constant density $1/(U - L)$ at points in the interval $[L, U]$ and density zero outside $[L, U]$.

Let X be a random variable with the uniform distribution between L and U. Then X has the following features:

$$\tilde{P}(X = t) = \begin{cases} \text{if } L \leq t \leq U & 1/(U - L) \\ \text{else} & 0 \end{cases}$$

$$P(X \leq t) = \begin{cases} \text{if } t \leq L & 0 \\ \text{if } L < t < U & (t - L)/(U - L) \\ \text{if } U \leq t & 1 \end{cases}$$

$$\text{Exp}(X) = \frac{U + L}{2}$$

$$\text{Var}(X) = \frac{(U - L)^2}{12}$$

The uniform distribution has a natural generalization to regions in $\mathbb{R}^k$. Let R be a bounded region in $\mathbb{R}^n$ whose volume is greater than zero. Then the uniform distribution over R has density $1/\text{volume}(R)$, where volume is the k-dimensional volume. If X is uniformly distributed over R then, for any measurable subset $S \subset R$, $P(X \in S) = \text{measure}(S)/\text{measure}(R)$.

The uniform distribution is the natural distribution to assume if an event is known to lie within a given region. For instance, if it is known that a meteor fell somewhere in the state of Michigan, but no information is available about where, then it is reasonable to assign the event a uniform distribution over the extent of Michigan.

The uniform distribution over [0,1] is also important computationally because it is easy to generate. To generate a 32-bit approximation of the uniform distribution between 0 and 1, just construct the number $0.b_1b_2 \ldots b_{32}$ where each bit b_i has 1/2 probability of being 0 or 1. If you want to generate random numbers corresponding to some other distribution, the usual procedure is to generate a uniform distribution and then apply a function to turn it into a different distribution.

9.8.2 The Gaussian distribution

The *Gaussian* or *normal* distribution is the most commonly used continuous distribution. It arises in all kinds of contexts and applications.

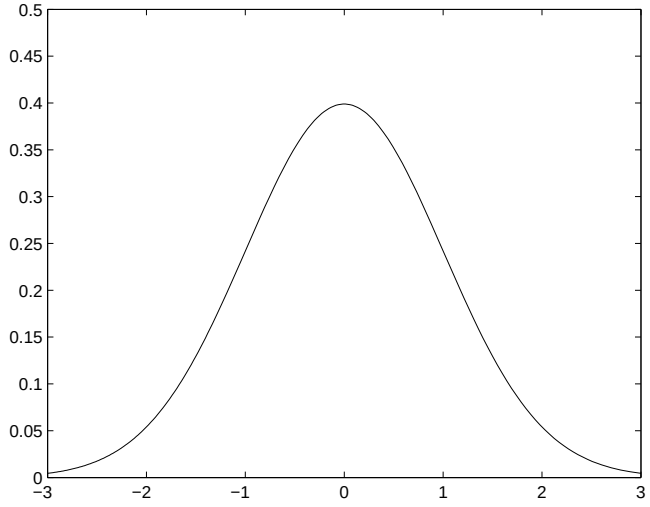


Figure 9.9: Gaussian density function

The Gaussian distribution has two parameters: the mean μ and the standard deviation σ. The density function denoted $N_{\mu,\sigma}(t)$ is shown in figure 9.9. It is defined as follows:

$$N_{\mu,\sigma}(t) = \frac{1}{\sqrt{2\pi}\sigma} e^{-t^2/2\sigma^2}$$

The denominator $\sqrt{2\pi} \cdot \sigma$ is just a normalizing factor. The density function is known as the "bell curve" because of its shape. It is symmetric around the mean μ; that is, for any x, $N_{\mu,\sigma}(\mu + x) = N_{\mu,\sigma}(\mu - x)$. It stays fairly flat within one standard deviation of μ; then it drops off rapidly going from 1 to 2 standard deviations; then it approaches 0 asymptotically very rapidly. Specifically:

$$\begin{aligned}
N_{\mu,\sigma}(\mu + 0.5\sigma) &= 0.88 \cdot N_{\mu,\sigma}(\mu). \\
N_{\mu,\sigma}(\mu + \sigma) &= 0.60 \cdot N_{\mu,\sigma}(\mu). \\
N_{\mu,\sigma}(\mu + 1.5\sigma) &= 0.32 \cdot N_{\mu,\sigma}(\mu). \\
N_{\mu,\sigma}(\mu + 2\sigma) &= 0.135 \cdot N_{\mu,\sigma}(\mu). \\
N_{\mu,\sigma}(\mu + 2.5\sigma) &= 0.0439 \cdot N_{\mu,\sigma}(\mu). \\
N_{\mu,\sigma}(\mu + 3\sigma) &= 0.01 \cdot N_{\mu,\sigma}(\mu). \\
N_{\mu,\sigma}(\mu + 4\sigma) &= 0.0003 \cdot N_{\mu,\sigma}(\mu). \\
N_{\mu,\sigma}(\mu + 5\sigma) &= 0.000004 \cdot N_{\mu,\sigma}(\mu).
\end{aligned}$$

Likewise, most of the distribution lies within 2 standard deviations of the mean, and virtually all of it lies within 3 standard deviations. Specifically, if X follows the distribution $N_(\mu, \sigma)$ then

$$\begin{aligned}
P(\mu - 0.5\sigma \leq X \leq \mu + 0.5\sigma) &= 0.38 \\
P(\mu - \sigma \leq X \leq \mu + \sigma) &= 0.68 \\
P(\mu - 1.5\sigma \leq X \leq \mu + 1.5\sigma) &= 0.86 \\
P(\mu - 2\sigma \leq X \leq \mu + 2\sigma) &= 0.95 \\
P(\mu - 2.5\sigma \leq X \leq \mu + 2.5\sigma) &= 0.987 \\
P(\mu - 3\sigma \leq X \leq \mu + 3\sigma) &= 0.997 \\
P(\mu - 4\sigma \leq X \leq \mu + 4\sigma) &= 1 - 6.3 * 10^{-5} \\
P(\mu - 5\sigma \leq X \leq \mu + 5\sigma) &= 1 - 5.7 * 10^{-7}
\end{aligned}$$

Thus, an event three standard deviations from the mean is rare (3 in 1000); four standard deviations is very rare (less than one in 10,000); five standard deviations is almost unheard of (less than one in 10,000,000).

If X follows the Gaussian distribution with mean μ and standard deviation σ, then variable $aX + b$ follows the Gaussian distribution with mean $a\mu + b$ and standard deviation $a\sigma$. In particular, the variable $Y = (X - \mu)/\sigma$ follows the distribution $N_{0,1}$. Therefore, if we have the cumulative distribution of $N_{0,1}$,

$$Z(t) = \int_{-\infty}^{t} N_{0,1}(u)du = \int_{-\infty}^{t} \frac{1}{\sqrt{2\pi}} e^{-u^2/2} du$$

as a built-in function (or in ye olden days when I was young, as a table in a book), we can compute $P(c \leq X \leq d) = P((c-\mu)/\sigma \leq Y \leq (d-\mu)/\sigma) = Z((d-\mu)/\sigma) - Z((c-\mu)/\sigma)$

The Gaussian distribution has the remarkable property that, if two independent random variables each follow a Gaussian, then their sum also follows a Gaussian.

Theorem 9.13. *Let X be a random variable whose density function is the Gaussian with mean μ_x and variance σ_x^2 and let Y be an independent random variable whose density function is the Gaussian with mean μ_y and variance σ_y^2. Then the density function of $X + Y$ is the Gaussian with mean $\mu_x + \mu_y$ and with variance $\sigma_x^2 + \sigma_y^2$.*

One of the main reasons that the Gaussian distribution is important is because of the central limit theorem:

Theorem 9.14. *(Central Limit Theorem). Let $X_1 \ldots X_n$ independent random variables, each of which has with mean μ and standard deviation σ. Let $Y = (X_1 + \ldots + X_n)/n$ be the average; thus Y has mean μ and standard deviation $\sigma/\sqrt{n}$. If n is large, then the cumulative distribution of Y is very nearly equal to the cumulative distribution of the Gaussian with mean μ and standard deviation σ_n.*

One particular, important, example is the binomial distribution. Suppose $X_1 \ldots X_n$ are independent and all have the Bernoulli distribution with parameter p. Then the sum $S = (X_1 + \ldots + X_n)/$ has the binomial distribution $B_{n,p}$. The X_i have mean $\mu = p$ and standard deviation $\sigma = \sqrt{p(1-p)}$. Let $Y = S/n$ be the average of the X_i. By the central limit theorem, the cumulative distribution of Y is very nearly equal to the cumulative distribution of the Gaussian with mean μ and standard deviation $\sigma/\sqrt{n}$. Therefore we can approximate the probability $P(c \leq Y \leq d)$ as the integral of $N_{\mu,\sigma}$ from c to d, and therefore, as discussed above, as $Z((d-\mu)/\sigma) - Z(c-\mu)/\sigma)$ where Z is the integral of the standard Gaussian, $Z(t) = \int_{-\infty}^{t} N_{0,1}(t)$.

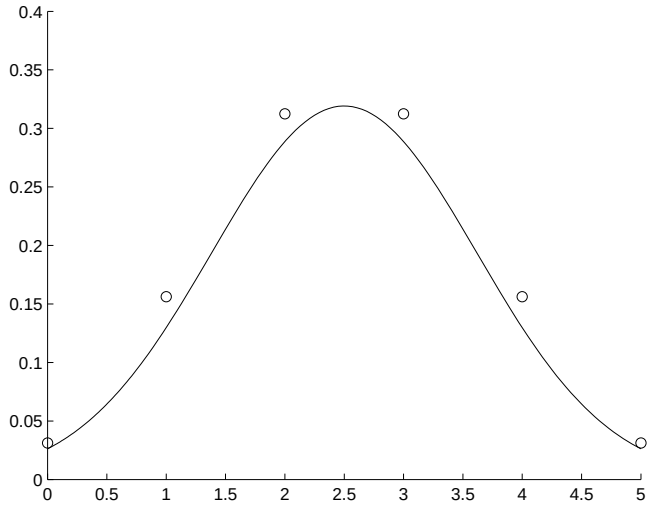
Likewise, the binomial distribution $B_{n,p}$ is very well approximated by the Gaussian density $N(\mu, \sigma)$ with a scaling factor of σ where $\sigma = \sqrt{p(1-p)n}$ (figure 9.10). Specifically,[7] for any fixed p, for all k,

$$|B_{n,p}(k) - \frac{N_{np,\sigma}(k)}{\sigma}| \text{ is } O(\frac{1}{n}).$$

(For the unique value $p = 1/2$, this is $O(1/n^{3/2})$.)

It should be noted that both of these approximations state only that the *difference* between the two functions is small. They do not state that the *ratio* is small, in the case where they are both close to zero. For example, in our discussion of the Zipf function, we mentioned estimates for the values $B_{n,p}(1)$ and of $B_{n,p}(6 * 10^6)$ where $p = 10^{-6}$ and $n = 10^8$. If you try to use the Gaussian as an estimate for the binomial distribution at these extreme values, you will not get an accurate answer.

[7] Thanks to Gregory Lawler for these bounds.



The green dots are the binomial distribution $B_{5,0.5}$
The red connected curve is the scaled Gaussian $N_{2.5,\sigma}/\sigma$, where $\sigma = \sqrt{5}/2$.
For values of n larger than 5, the fit is even closer.

Figure 9.10: Gaussian density function

9.9 MATLAB

The computation of the functions associated with discrete numerical random variables presents no particular new issues, and MATLAB provides few utilities particularly tailored to these computations. The function `nchoosek(N,K)` computes the binomial coefficient $N!/K!(N-K)!$.

```
>> nchoosek(5,2)
ans =
    10
>> nchoosek(10,5)
ans =
   252
```

For computations with continuous distributions, there are two important MATLAB functions: the general function for computing integrals, and the specific function for the integral of the Gaussian.

A definite integral in MATLAB can be computed using the function `quad(fn,a,b)` where `fn` is a specification of the integrand, a is the lower bound, and b is the upper bound. There are a number of ways to write the integrand `fn`. The simplest is as follows; write a MATLAB expression $\alpha(v)$ where v corresponds to a vector of values of t $\langle t_1 = a \ldots t_n = b \rangle$ and $\alpha(v)$ corresponds to the vector $\langle f(t_1) \ldots f(t_n) \rangle$. Then stick $\alpha(v)$ between single quotation marks. The expression should contain only one variable, which is the variable being integrated over. (The support for functional programming in MATLAB is mediocre.)

For instance you can evaluate the integral of $1/(1+t^2)$ from 1 to 2 as follows:

```
>> quad('1./(1+v.^2)',1,2)
```

```
ans =
   0.3218
```

The cumulative distribution function of the standard Gaussian $\int_{-\infty}^{x} N_{0,1}(t)dt$ is not an elementary function; that is, it is not expressible as a combination of polynomials, logs, exponentials, and trigonometric functions. However, there is a built-in MATLAB function `erf(x)` that computes a closely related function called the *error function*. The error function is defined as follows:

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

Therefore the total weight of the standard Gaussian in an interval $[-x, x]$ symmetric around 0 can be computed as

$$\int_{-x}^{x} \frac{1}{\sqrt{2\pi}} e^{-u^2/2} du = \int_{-x/\sqrt{2}}^{x/\sqrt{2}} \frac{1}{\sqrt{\pi}} e^{-t^2} dt = \int_0^{x/\sqrt{2}} \frac{2}{\sqrt{\pi}} e^{-t^2} dt = \text{erf}(x/\sqrt{2})$$

The first transformation follows from substituting $t = u/\sqrt{2}$. The second follows from the fact that the integrand is symmetric around 0.

The cumulative distribution of the standard Gaussian can be computed as

$$\int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{-u^2/2} du = \int_{-\infty}^{x/\sqrt{2}} \frac{1}{\sqrt{\pi}} e^{-t^2} dt = \int_{-\infty}^{0} \frac{1}{\sqrt{\pi}} e^{-t^2} dt + \int_0^{x/\sqrt{2}} \frac{1}{\sqrt{\pi}} e^{-t^2} dt = \frac{1}{2}(1 + \text{erf}(x/\sqrt{2}))$$

(The function erf does the right thing here for negative values of x.)

The MATLAB function `erfinv(y)` computes the inverse of erf

Therefore

```
% To compute the probability that a normal distribution is within
% 1.6 standard deviations of the mean
>> erf(1.6/sqrt(2))
ans =
   0.8904

% To compute the probability that a normal distribution is less than
% mu + 1.6 sigma, where mu is the mean and sigma is the standard deviation
>> (1+erf(1.6/sqrt(2)))/2
ans =
   0.9452

% To find the value of d such that X is between mu-d*sigma and mu+d*sigma
% with probability 0.8
>> erfinv(0.8)*sqrt(2)
ans =
   1.2815
```

Exercises

Exercise 9.1

Let X be a random variable with values -1, 2, 6, such that $P(X = -1) = 0.2, P(X = 2) = 0.5, P(X = 6) = 0.3$. Compute $\text{Exp}(X), \text{Var}(X), \text{Std}(X)$.

Exercise 9.2

Let X be a random variable with values 0, 1 and 3 and let Y be random variable with values -1, 1, 2, with the following joint distribution:

X\Y	-1	1	2
0	0.12	0.08	0.10
1	0.20	0.04	0.25
3	0.08	0.10	0.05

A. Compute the marginal distributions.
B. Are X and Y independent? Justify your answer.
C. Compute $\text{Exp}(X)$ and $\text{Exp}(Y)$.
D. Compute the distribution of $X + Y$.
E. Compute $P(X|Y = 2)$ and $P(Y|X = 1)$.

Exercise 9.3

Let X be a random variable with values 0, 1, and 3 and let Y be random variable with values -1, 1, 2. Suppose that $P(X = 1) = 0.5, P(X = 2) = 0.4$, and $P(X = 3) = 0.1$; and that the values of $P(Y|X)$ are given in the following table:

X\Y	-1	1	2
0	0.5	0.3	0.2
1	0.2	0.7	0.1
3	0.4	0.1	0.5

A. Compute the joint distribution of X, Y.
B. Compute the distribution of Y.
C. Compute the corresponding table for $P(X|Y)$.
D. Compute the distribution of $X + Y$.
E. Compute $\text{Exp}(X)$, $\text{Exp}(Y)$ and $\text{Exp}(X + Y)$.

Problems

Problem 9.1

(You may use MATLAB).

A patient comes into a doctors office exhibiting two symptoms: s1 and s2. The doctor has two possible diagnoses: disease d1 or disease d2. Assume that, given the symptoms, the patient must have either d1 or d2, and cannot have both. We are given the following probabilities:

P(s1 | d1) = 0.8.
P(s1 | d2)= 0.4.
P(s2 | d1)= 0.2.
P(s2 | d2)= 0.6.
P(d1) = 0.003.
P(d2) = 0.007.

Assume that s1 and s2 are conditionally independent given the disease.

A. What are P(d1 | s1,s2) and P(d2 | s1,s2)?

B. The doctor has the choice of two treatments, t1 and t2. (It is not an option to do both.) Let c be the event that the patient is cured. We are given the following probabilities:

P(c | d1,t1) = 0.8
P(c | d2,t1) = 0.1
P(c | d1,t2) = 0.3
P(c | d2,t2) = 0.6

Assume that the event c is conditionally independent of the symptoms, given the disease and the treatment. What is P(c | t1,s1,s2)? What is P(c | t2,s1,s2)?

C. Suppose that treatment t1 has cost \$1000 and treatment t2 has cost \$500. If the patient has disease d1, then the value of being cured is \$20,000; if the patient has disease d2, then the value of being cured is \$15,000. Given that the patient is exhibiting symptoms s1 and s2, what is the expected value of applying t1? What is the expected value of applying t2?

D. The doctor also has the option of ordering a test with a Boolean outcome. The test costs \$800. Logically, tests are like symptoms, so let event s3 be a positive result on this test. We are given the following probabilities:

P(s3 | d1) = 0.9
P(s3 | d2) = 0.1

Assume that s3 is conditionally independent of s1 and s2 given the disease. Is it worthwhile ordering the test? What is the expected gain/cost from ordering the test?

Problem 9.2

(You may use MATLAB)

Let us continuing the example of the publisher and the reviewer discussed in section 9.3.2. Suppose that the publisher also has the option of consulting with two reviewers. Assume that the two reviewers follow the same probabilistic model, and that their reviews are conditionally independent given the actual success or failure.

A. Consider the following possible strategies:

1. Consult with one reviewer,
2. Consult with two reviewers. If both approve the manuscript, then publish, otherwise reject.
3. Consult with two reviewers. If either approves the manuscript, then publish, otherwise reject.

Suppose that a reviewer's fee is \$500. Add these options to the decision tree in figure 9.3. What are the expected values of these strategies? Which is the optimal strategy?

Problem 9.3

Continuing problem 9.2: If the publisher has enough time, it may be possible to delay deciding whether to consult the second reviewer until the opinion of the first is known. This allows two more possible strategies.

- Consult reviewer A. If his opinion is favorable, consult reviewer B. If both are favorable, publish.
- Consult reviewer A. If his opinion is unfavorable, consult reviewer B. If either is favorable, publish.

A. Add these to the decision tree in problem 9.2. What are the expected values of these strategies? What is the optimal strategy.

B. (Difficult). Present an argument that any other strategy besides the four we have considered is either obviously inferior or essentially equivalent. Your argument should be independent of the specific values of the probabilities, costs, and benefits involved; however, you should assume that reviewers A and B are equally accurate and equally expensive.

Problem 9.4

Let M be a matrix representing the joint distribution of two random variables X, Y, as in table 9.1. Prove that if X and Y are independent, then $\text{Rank}(M) = 1$.

Problem 9.5

Let X be a numerical random variable. A value q is defined as a *median* of X if $P(X > q) \leq 1/2$ and $P(X < q) \leq 1/2$. (A random variable may have more than one median). Show that, for any random variable X with finitely many values, any value of v that minimizes the expression $\text{Exp}(|X - v|)$ is a median of X. (This is stated without proof on p. 232. The statement is true also for numerical random variables with infinitely many values, but the proof is more difficult.)

Hint: Consider how the value of $\text{Exp}(|X - v|)$ changes when v is moved slightly in one direction or the other. Some experimentation with a simple example may be helpful.

Programming assignments

Assignment 9.1

Random variable X takes on integer values from 1 to 500 and obeys an inverse power-law distribution with exponent 2.28. That is, $P(X = k) = \alpha/k^{2.28}$ for some constant α.

A. Find α. (Hint: the probabilities must sum to 1.)
B. Find $\text{Exp}(X)$.
C. Find $\text{Std}(X)$.

D. (Difficult: Requires some familiarity with infinite series). Consider a variable Y which obeys the same power-law distribution as X, but takes on integer values from 1 to ∞. Estimate the accuracy

of the values you have computed in parts A, B, C, as approximations for the corresponding values for Y.

Assignment 9.2

This assignment is a generalization of problems 9.2 and 9.3. As in those problems, there is a publisher who needs to decide whether to publish a book, and who has the option of consulting with a number of reviewers. The outcome of publishing is either Success, with a specified profit, or Fail with a specified loss. The outcome of not publishing is 0. Consulting with a reviewer costs a specified amount. A reviewer gives a Boolean answer, For or Against. Reviewers' opinions are conditionally independent given the value of Success/Fail.

A. Write a MATLAB function

```
PubValue(Profit,Loss,Fee,ProbSuc,ProbForSuc,ProbForFail,N)
```

This takes the following arguments:

`ValueSuc` = Dollar profit if the book succeeds.
`ValueFail` = Dollar profit if the book fails.
`Fee` = Cost of hiring a reviewer.
`ProbSuc` = P(Success).
`ProbForSuc` = P(For | Success).
`ProbForFail` = P(For | Fail).
`N` = Number of reviewers consulted. May be 0.

The function returns the expected profit to the publisher, assuming that N reviewers are consulted.

B. Write a MATLAB function

```
OptimalN(Profit,Loss,Fee,ProbSuc,ProbForSuc,ProbForFail)
```

which returns a pair of values: The optimal number of reviewers to consult, and the expected value.

Assignment 9.3

Consider the following simple model for disease diagnosis. We make the following assumptions:

- There are N possible symptoms (including test results) which in this problem we will take, unrealistically, to be Boolean – i.e. you either have the symptom or you don't; the test either succeeds or fails.
- There are M diseases under consideration.
- Symptoms are conditionally independent given the disease.
- Any patient has exactly one diagnosis.
- There are Q different treatments. A patient can be given a single treatment. We will similarly assume, unrealistically, that the effectiveness of a treatment is Boolean; either a treatment entirely cures the disease or it is useless.

The *symptom matrix* is an $M \times N$ matrix S of probabilities: $S[I, J] = P(J|I)$, the probability that a patient exhibits symptom J given that he has disease I.

Part A

A *patient record* is a Boolean vector of length N indicating the patient's symptoms. Write a function `RecProb(R,S)` that takes as arguments a patient record `R` and a symptom matrix `S` and returns a vector `D` of length M such that $D[I] = P(R|I)$ for each disease I.

Part B

The *frequency* vector is a vector `F` of length M such that `F[I]` is the frequency of disease `I` in the population at large. Write a function `Diagnose(R,S,F)` which returns a vector `D` of length M such that `D[I]` = `P(I|R)`, the probability that a patient with symptoms `R` has disease `I`. Use Bayes' law. Include the normalizing factor.

Part C

A *treatment efficacy* matrix is a $Q \times M$ matrix `T` where `T[I, J]` is the probability that treatment `I` will cure disease `J`. Assume that the event that I cures J is independent of the event that J manifests symptom K; that is, given that a patient has a particular disease, the effectiveness of the treatment is not affected by the particular symptoms he is manifesting. Write a function `Prognosis(R,S,F,T)` which returns a vector `W` of length Q, where `W[I]` is the probability that a patient with symptoms `R` will be cured of his disease by treatment `I`.

Part D

A *disease cost vector* is a vector `C` of length M indicating the cost of leaving disease `I` uncured. (We will assume that this depends on the disease, rather than on the symptoms.) A *treatment cost vector* is a vector `B[I]` of length Q, where indicating the cost of attempting treatment `I`. (Of course, for both of these, "cost" should be interpreted broadly as including all the undesirable consequences.) Write a function `Benefit(R,S,F,T,C,B)` which returns a vector `A` where `A[I]` is the expected benefit of applying treatment `I` to a patient with symptoms `R`. Note that the benefit of curing the disease applies only if the disease is cured, whereas the cost of the treatment applies whether or not the disease is cured.

Assignment 9.4

In this part you will redo parts A and B of assignment 9.3 on the more realistic assumption that symptoms are numeric rather than Boolean, and the (common but often very unrealistic) assumption that each symptom is normally distributed. Specifically: Assume that all symptoms are numeric though diseases continue to be Boolean; that is, ignore the difference between a mild case and a severe case of the disease. Let `S` now be an $M \times N$ array, such that, for any disease `I` and symptom `J`, the measure x of symptom `J` given that the patient has disease `I` is normally distributed with mean `S[I, J]` and standard deviation 1; that is, it follows the distribution $N_{\mathtt{S[I,J]},\sigma}(x) = \exp(-(x - \mathtt{S[I,J]})^2/2)/\sqrt{2\pi}$.

Part A

Write a function `RecProbN(R,P)` that takes as arguments a patient record `R` and a symptom matrix `S` and returns a vector `D` of length M such that `D[I]` = $\tilde{P}$`(R|I)` for each disease I.

Part B

The *frequency* vector is a vector `F` of length M such that `F[I]` is the frequency of disease `I` in the population at large. Write a function `Diagnose(R,S,F)` which returns a vector D of length M such that `D[I]` $= P($`I`$|$`R`$)$, the probability that a patient with symptoms `R` has disease `I`.

Chapter 10

Markov Models

Markov models, also known as a *Markov chains* or *Markov processes* are a type of probabilistic model which are very useful in the analysis of strings or sequence, such as text or time series.

In a Markov process, time is viewed discretely; time instants are numbered 0, 1, 2 .... The process has a finite[1] number of *states;* at each instant, the process is in one particular state. Between time I and time $I + 1$, the process executes a *transition* from one state to another; its destination is probabilistically determined. The key property of a Markov process is that the probability of the transition depends only on the current state, and not on any of the previous state. That is, so to speak, whenever you are in a state, you spin a wheel of fortune which tells you where to go next. Each state has its own wheel, but the wheel at a given state remains constant over time, and the choice of where to move next depends only on the outcome of the wheel spin and on nothing else. This is known as the "Markov condition". It is sometimes described by saying that the system is memoryless and time-invariant; what it does next depends only on where it is now, and not on how it got there, or on what time it is.

A simple example of a Markov model is the children's board game "Chutes and Ladders".[2] In this game, the board has 100 squares in sequence; there are a number of "ladders" which take you forward to a more advanced square and a number of "chutes" which take you back to an earlier square. Each player rolls a die and moves forward the number of squares shown on the roll. If he ends at the bottom of a ladder, he climbs it; if he ends at the top of a chute, he slides down.

For a single player, the corresponding Markov model has a state for every possible resting square (i.e. square that is not the bottom of a ladder or the top of a chute.) Each state has 6 transitions, each with probability 1/6, corresponding to the 6 possible outcomes of the die roll. Figure 10.1 shows the Markov model corresponding to a simplified game in which there are only 6 resting squares and in which the die has only two outcomes, 1 and 2. Each of the arcs has the label 1/2, except for the final self-loop from S6 to itself, which has label 1.

In a game on the same board with k players are taking turns, a state is a $k+1$ tuple $S = \langle s_1 \ldots s_k, p \rangle$ where s_i is the location of player i and p is an index from 1 to k indicating which player moves next. For example, if 3 players play the game in figure 10.1 then one state is $\langle$S5, S3, S3, 2 $\rangle$. This has two transitions, each with probability 1/2: one to $\langle$ S5, S2, S3, 3 $\rangle$ and the other to $\langle$ S5, S4, S3, 3 $\rangle$.

We can describe a Markov model in terms of random variables. For each time instant, $t = 0, 1, 2 \ldots$,

[1] One can also define Markov processes with infinitely many states; however, we will not consider these in this book.

[2] The example is from Philip J. Davis and William G. Chinn, *3.1416 and all that,* 2nd edn, Boston: Birkhauser 1985.

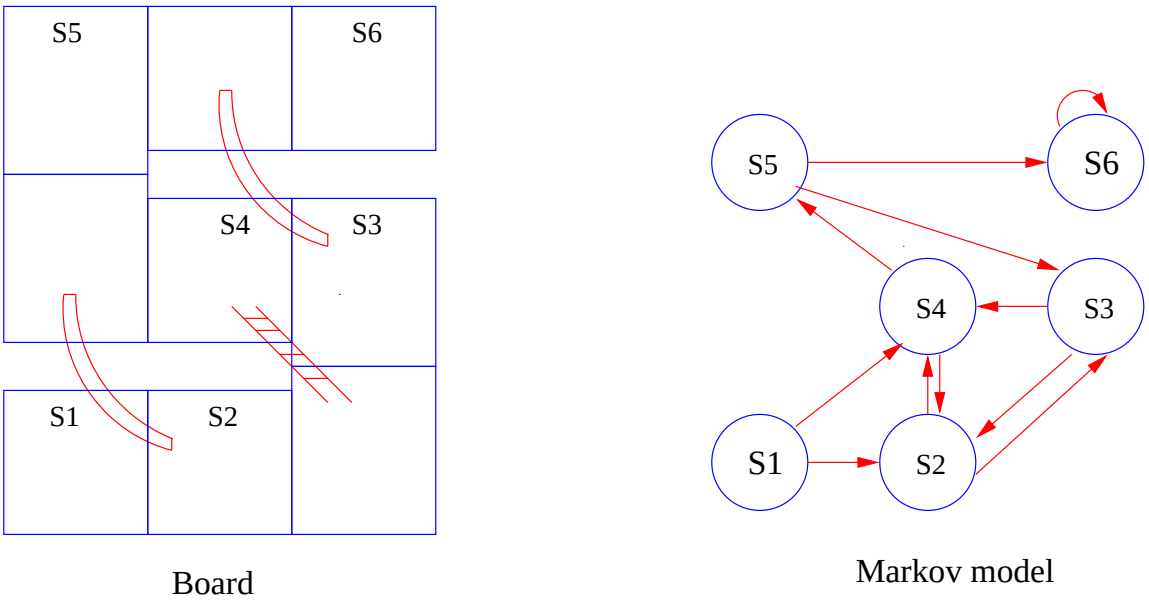


Figure 10.1: Chutes and Ladders: Markov Model

we define the random variable X_t to be the state of the system at time t. Thus, the domain of values for X_i is the set of states of the Markov model. The conditional probability $P(X_{t+1} = u \,|X_t = v)$ is the label on the arc in the model from u to v. The condition that the model is memoryless corresponds to the statement that X_{t+1} is conditionally independent of $X_1 \ldots X_{t-1}$ given X_t. The condition that the model is time-invariant corresponds to the statement that

$P(X_{t+1} = u \,|X_t = v) = P(X_{s+1} = u \,|X_s = v)$ for all times t and s.

Let us assign indexes $1 \ldots k$ to the k states of the model. Then we can view the probability distribution of X_t as a k-dimensional vector $\vec{X}_t$. We can also characterize the Markov model by a $k \times k$ *transition* matrix M where $M[i, j] = P(X_{t+1} = i \mid X_t = j)$. By the axioms of probability,

$$P(X_{t+1} = i) = \sum_{j=1}^{k} P(X_{t+1} = i, X_t = j) = \sum_{j=1}^{k} P(X_{t+1} = i \mid X_t = j) P(X_t = j)$$

This can be written as a matrix multiplication: $\vec{X}_{t+1} = M \cdot \vec{X}_t$.

For example, the Markov model in figure 10.1 has the following transition matrix:

$$M = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 1/2 & 0 & 0 \\ 0 & 1/2 & 0 & 0 & 1/2 & 0 \\ 1/2 & 1/2 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/2 & 1 \end{bmatrix}$$

If $\vec{X}_0 = \langle 1, 0, 0, 0, 0, 0 \rangle$ — that is, the player definitely starts at S1 at time 0, then

$$\begin{array}{lllllllllll} \vec{X}_1 & = & M \cdot \vec{X}_0 & = & \langle & 0, & 1/2, & 0, & 1/2, & 0, & 0 & \rangle. \\ \vec{X}_2 & = & M \cdot \vec{X}_1 & = & \langle & 0, & 1/4, & 1/4, & 1/4, & 1/4, & 0 & \rangle. \\ \vec{X}_3 & = & M \cdot \vec{X}_2 & = & \langle & 0, & 1/4, & 1/4, & 1/4, & 1/8, & 1/8 & \rangle. \\ \vec{X}_4 & = & M \cdot \vec{X}_3 & = & \langle & 0, & 1/4, & 3/16, & 1/4, & 1/8, & 3/16 & \rangle. \end{array}$$

A few points to notice about this. First, we have $\vec{X}_3 = M \cdot \vec{X}_2 = M \cdot M \cdot \vec{X}_1 = M \cdot M \cdot M \cdot X_0 = M^3 \cdot \vec{X}_0$; in general, we have $\vec{X}_n = M^n \cdot X_0$.

Second, each column of matrix M add up to 1. This corresponds to the fact that the transitions out of state j form a frame of discernment — exactly one transition occurs — so

$$\sum_{i=1}^{k} M_{i,j} = \sum_{i=1}^{k} P(X_{t+1} = i \mid X_t = j) = 1$$

A matrix with this feature is called a *stochastic* matrix. As a consequence, the sum of the values of $M \cdot \vec{v}$ is equal to the sum of the values of $\vec{v}$ for any $\vec{v}$.

Third, you may notice that the analysis here is oddly similar to application 13, of population transfer between cities, in section 3.4.1. In fact, it is exactly the same, with probability density here replacing population there. More precisely, that example was contrived as something that resembled a Markov process but did not require a probabilistic statement.

We will not explore the mathematics of Markov models in depth. Rather we focus on two computer science applications of Markov models: the computation of PageRank for web search, and the tagging of natural language text. First, we discuss the general issue of stationary distributions, which is needed for the analysis of PageRank.

10.1 Stationary probability distribution

Consider a Markov process with transition matrix M. A probability distribution $\vec{P}$ over the states of M is said to be *stationary* if $\vec{P} = M \cdot \vec{P}$. Thus, if $\vec{X}_t = \vec{P}$ then $\vec{X}_{t+1} = \vec{P}$; if you start with this probability distribution, then you stay with this probability distribution.

Theorem 10.1. *Every finite Markov process has a stationary distribution. Equivalently, for every stochastic matrix M there exists a probability distribution $\vec{P}$ such that $\vec{P} = M \cdot \vec{P}$.*

The example of Chutes and Ladders above is unfortunately not a very interesting example of this theorem; the unique stationary distribution is $\langle 0, 0, 0, 0, 0, 1 \rangle$. Let us therefore change the example by removing the self-arc from S6 to itself and replacing it with an arc from S6 to S1; when you have finished the game, you start at the beginning again. Figure 10.2 shows the revised Markov model. In that case, the stationary distribution is $\langle 1/15, 4/15, 3/15, 4/15, 2/15, 1/15 \rangle$, as is easily checked. (For checking by hand, notice that the property $\vec{P} = M \cdot \vec{P}$ remains true if you multiply through by a scalar, so you can ignore the denominator 15.)

In fact, most Markov models have exactly one stationary distribution. The following theorem gives a condition that suffices to guarantee that the stationary distribution is unique.

Definition 10.1. *Let G be a directed graph. G is* strongly connected*, if, for any two vertices u and v in G there is a path from u to v through G.*

Theorem 10.2. *Let M be a finite Markov model. Let G be the graph whose vertices are the states of M and whose arcs are the transitions with non-zero probability. If G is strongly connected then M has exactly one stationary distribution.*

Moreover, most Markov models have the property that, if you run them for long enough, they converge to the stationary distribution, whatever the starting distribution. The following theorem gives a condition that ensures that the distribution converges:

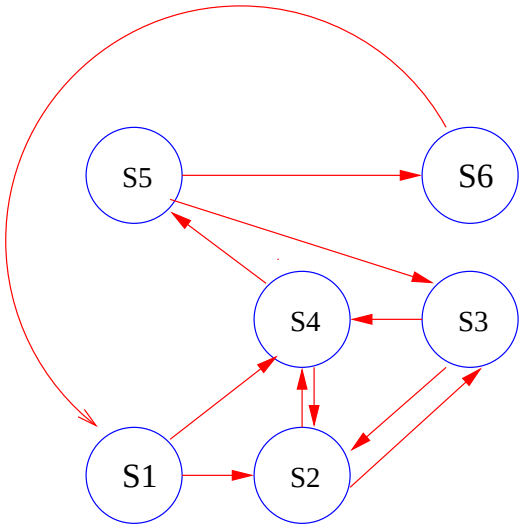


Figure 10.2: Modified Markov model

Definition 10.2. *Let G be a directed graph and let $k > 1$ be an integer. Vertex v in G is* periodic with period k *if every cycle from v to itself through G has a length divisible by k. G is* aperiodic *if no vertex in G is periodic for any period $k > 1$.*

Theorem 10.3. *Let M be a finite Markov model. Let G be the graph whose vertices are the states of M and whose arcs are the transitions with non-zero probability. If G is strongly connected and aperiodic then, for any starting distribution $\vec{X}_0$, the sequence $\vec{X}_0, M\vec{X}_0, M^2\vec{X}_0, \ldots$ converges to the stationary distribution.*

That is, if M satisfies the above condition, then however you start, if you run the model long enough, it converges to the stationary distribution $\vec{D}$. Thus, Markov models are "memoryless" in a second sense as well; over time, they entirely forget where they started from, and converge to a distribution that depends only on the transition matrix.

For example, let M be the modified model above, Then as stated above, the stationary distribution $\vec{D} = \langle 1/15, 4/15, 3/15, 4/15, 2/15, 1/15\rangle = \langle 0.0667, 0.2667, 0.2000, 0.2667, 0.1333, 0.0667\rangle$.
Let $\vec{X}_0 = \langle 1, 0, 0, 0, 0, 0\rangle$ (i.e. at time 0 you are definitely at S1). Then

$\vec{X}_4 = M^4 \cdot \vec{X}_0 = \langle 0.1250, 0.2500, 0.1875, 0.2500, 0.1250, 0.0625\rangle$
$\vec{X}_8 = M^8 \cdot \vec{X}_0 = \langle 0.0703, 0.2656, 0.1992, 0.2656, 0.1328, 0.0664\rangle$
$\vec{X}_{12} = M^{12} \cdot \vec{X}_0 = \langle 0.0669, 0.2666, 0.2000, 0.2666, 0.1333, 0.0667\rangle$
$|\vec{X}_{12} - \vec{D}| = 2.5 \cdot 10^{-4}$.

10.1.1 Computing the stationary distribution

Given a transition matrix M, the stationary distribution $\vec{P}$ can be computed as follows. The vector $\vec{P}$ satisfies the equations $M\vec{P} = \vec{P}$, and the equation $\sum_{I=1}^{n} \vec{P}[I] = 1$. We can rewrite the first equation as $(M - I_n) \cdot \vec{P} = \vec{0}$, where I_n is the identity matrix. For a Markov model with a unique stationary distribution, $M - I_n$ is always a matrix of rank $n - 1$. We can incorporate the final constraint $\sum_{I=1}^{N} \vec{P}[I] = 1$ by constructing the matrix Q whose first n rows are $M - I_n$ and whose last row is all 1's. This is an $(n + 1) \times n$ matrix of rank n. The vector $\vec{P}$ is the solution to the equation $Q \cdot \vec{P} = \langle 0, 0 \ldots 0, 1\rangle$.

For example suppose $M = [1/2, 2/3; 1/2, 1/3]$:

```
>> m=[1/2,2/3;1/2,1/3]
m =
    0.5000    0.6667
    0.5000    0.3333

>> q=m-eye(2)
q =
   -0.5000    0.6667
    0.5000   -0.6667

>> q(3,:)=[1,1]
q =
   -0.5000    0.6667
    0.5000   -0.6667
    1.0000    1.0000

>> q\[0;0;1]
ans =
    0.5714
    0.4286

>> m*ans
ans =
    0.5714
    0.4286
```

If the graph is large, there are more efficient, specialized algorithms.

10.2 PageRank and link analysis

The great Google empire began its existence as a project of Sergey Brin and Lawrence Page, then two graduate students at Stanford, aimed at improving the quality of search engines.[3] Their idea,[4] described in the now classic paper "The PageRank Citation Ranking" was as follows. The ranking of a web page P to a query Q consists of two parts. First, there is a *query-specific* measure of relevance – how well does this page match the query? This is determine by the vector theory of documents or something similar (see assignment 2.1, chapter 2). Second, there is a *query-independent* measure of the quality of the page – how good a page is this, overall? This latter measure, in the PageRank theory, is measured using link analysis. Previous to Google, it appears that search engines used primarily or exclusively a query-specific measure. This could lead to anomalies. For example, Brin

[3]Readers who had not been using search engines prior to Google may not realize how thoroughly it revolutionized the field. The earliest web search engines were introduced in 1993, and search engines such as Infoseek (launched 1994) and AltaVista (lauched 1995) soon became widely used and were initially quite effective. By 1998, however, the quality of results returned by these search engines was visibly deteriorating; the ranking algorithms simply could not keep up with the exponential growth in the Web. When Google was released, the improvement in quality was startling.

[4]The ranking method now used by Google, though highly secret, is clearly much more complex than the theory below. The current ranking system certainly makes heavy use of user logs, which were hardly available when Google was first launched. However, unquestionably link-based measures are still an important component of the current ranking method.

and Page mention that, at one point, the top page returned by one of the search engines to the query "Bill Clinton" was a page that said, simply, "Bill Clinton sucks." Why not? After all, 2/3 of the words on the page match words in the query; that would be hard to beat.

The first idea is that, if a page P is good, then many people will have linked to it. So one measure of quality would be just the number of in-links to a page P. However (2nd idea) some links are more important than others. For example:

1. Links from a different web site, which indicate an outside interest, should count more than links from same domain, which just indicate the structure of the web site.
2. Characteristics of anchor (e.g. font, boldface, position in the linking page) may indicate a judgement by the author of the linking page of relative importance of P.
3. A link from an important page is more important than a link from an unimportant page. This is circular, but the circularity can be resolved.

The PageRank algorithm works with idea (3) above. Suppose that each page P has an importance $I(P)$ computed as follows: First, every page has an inherent importance E (a constant) just because it is a web page. Second, if page P has importance $I(P)$ then P contributes an indirect importance $F * I(P)$ that is shared among the pages that P points to. (F is another constant). That is. let $O(P)$ be the number of outlinks from P. Then if there is a link from P to Q, then P contributes $F * I(P)/O(P)$ "units of importance" to Q.

(What happens if P has no outlinks, so that $O(P) = 0$? This actually turns out to create a little trouble for our model. For the time being, we will assume that every page has at least one outlink, and we will return to this problem below.)

We therefore have the following equation: for every page Q, if Q has in-links from $P_1 \ldots P_m$ then

$$I(Q) = E + \frac{F \cdot I(P_1)}{O(P_1)} + \ldots + \frac{F \cdot I(P_m)}{O(P_m)} \tag{10.1}$$

Thus, we have a system of n linear equations in n unknowns, where n is the number of web pages.

We now make the following observation. Suppose we write down all the above equations for all the different pages Q on the Web. Now add all the equations. On the left we have the sum of $I(Q)$ over all Q on the web; call this sum S. On the right we have N occurrences of E and for every page P, O_P occurrences of $F * I(P)/O_P$. Therefore, over all the equations, we have for every page P a total of $F \cdot I(P)$, and these add up to FS. Therefore, we have

$$S = NE + FS \text{ so } F = 1 - NE/S \tag{10.2}$$

Since the quantities E, F, N, S are all positive, it follows that $F < 1, E < S/N$.

We can normalize this as follows: Let $J(Q) = I(Q)/S$ and let $e = E/S$. Then the above equations become:
$J(Q) = e + F * (J(P_1)/O(P_1) + \ldots + J(P_m)/O(P_m))$ and
$1 = Ne + F$.

For example suppose we have pages U,V,W,X,Y,Z linked as shown in figure 10.3.

Note that X and Y each have three in-links but two of these are from the "unimportant" pages U and W. Z has two in-links and V has one, but these are from "important" pages. Let $e = 0.05$ and let F=0.7. We get the following equations (for simplicity, I write the page name rather than J(page name)):

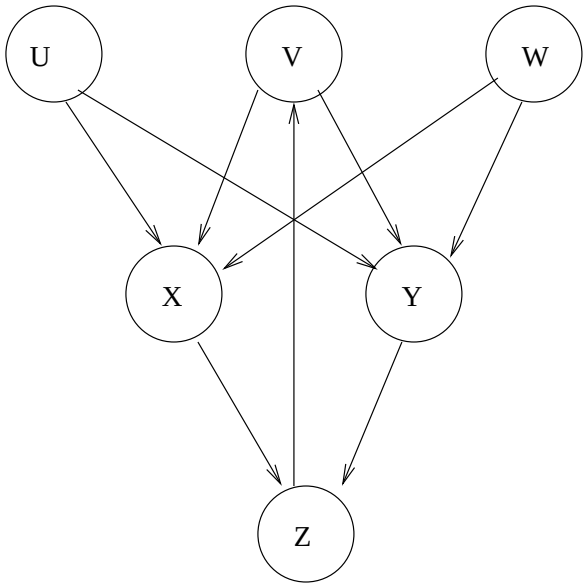


Figure 10.3: Link analysis for web pages

```
U = 0.05
V = 0.05 + 0.7 * Z
W = 0.05
X = 0.05 + 0.7*(U/2+V/2+W/2)
Y = 0.05 + 0.7*(U/2+V/2+W/2)
Z = 0.05 + 0.7*(X+Y)
```

The solution to these is U = 0.05, V = 0.256, W = 0.05, X = 0.175, Y = 0.175, Z = 0.295

10.2.1 The Markov model

We can turn the above system of equations into a stochastic system of equations as follows. First let $\vec{J}$ be the N-dimensional vector where $\vec{J}[Q] = J(Q)$; thus $\sum_{Q=1}^{N} \vec{J}[Q] = 1$, so $\vec{J}$ is a probability distribution. Now let M be the $N \times N$ matrix such that

$$M[P,Q] = \begin{cases} e + \frac{F}{O(Q)} & \text{if } Q \text{ points to } P \\ e & \text{if } Q \text{ does not point to } P \end{cases}$$

Then for each column Q, $\sum_P M[P,Q] = \sum_{P=1}^{N} e + \sum_{P|Q\to P} F/O(Q) = Ne + F = 1$, so M is a stochastic matrix.

Moreover, for each row P,

$$\sum_{Q=1}^{N} M[P,Q]\vec{J}[Q] = \sum_{Q=1}^{N} e\vec{J}[Q] + \sum_{Q\to P} \frac{F}{(O(Q))}\vec{J}[Q] =$$

$$e \cdot \sum_{Q=1}^{N} \vec{J}[Q] + \sum_{Q\to P} \frac{F}{O(Q)} \cdot J(Q) = e + \sum_{Q\to P} F \cdot \frac{J(Q)}{O(Q)} = \vec{J}[P]$$

In other words $M\vec{J} = \vec{J}$, so $\vec{J}$ is the stationary distribution for M.

M then corresponds to the Markov model where there is a link from every page Q to every page P (including self-link). The probability of the link is e if Q does not point to P and is $e + F/O(Q)$ if Q does point to P. We can view this in terms of the following stochastic model: Imagine someone who is browsing the web for a very long time. Each time he reads a page P, he decides where to go next using the following procedure:

1. Flip a weighted coin, that comes up heads with probability F and tails with probability $1 - F$.
2. If the coin comes up heads, he picks an outlink from P at random and follows it. (Again, we assume that every page has at least one outlink.)
3. If the coin comes up tails, he picks a page at random in the Web and goes there.

In the above example above, $F = 0.7, e = (1 - 0.7)/6 = 0.05$ so M is the matrix

$$\begin{bmatrix} 0.05 & 0.05 & 0.05 & 0.05 & 0.05 & 0.05 \\ 0.05 & 0.05 & 0.05 & 0.05 & 0.05 & 0.75 \\ 0.05 & 0.05 & 0.05 & 0.05 & 0.05 & 0.05 \\ 0.40 & 0.40 & 0.40 & 0.05 & 0.05 & 0.05 \\ 0.40 & 0.40 & 0.40 & 0.05 & 0.05 & 0.05 \\ 0.05 & 0.05 & 0.05 & 0.75 & 0.75 & 0.05 \end{bmatrix}$$

Since the graph is fully connected, theorem 10.2 applies, and there exists a unique stationary distribution.

From a computational point of view, this would at first seem to be a step in the wrong direction. We have turned an extremely sparse system of equations into an entirely dense one; moreover, with N equal to several billion, the transition matrix cannot even be generated or stored, let alone used in calculation. However, it turns out that, because of the special form of this matrix, there are fast iterative algorithms known for computing the stationary distribution. See (Langville and Meyer 2006).

Also note that the connection to Markov processes is actually bogus; the justification of the link analysis does not actually require any reference to any kind of random event or measure of uncertainty. The reasons to present this in terms of Markov models are, first, because the mathematics of stochastic matrices has largely been developed in the context of Markov models; second, because the stochastic model is a useful metaphor in thinking about the behavior of PageRank and in devising alternative measures.

In understanding the behavior of the algorithm, it is helpful to consider its behavior for different values of the parameter F. If $F = 0$ then the links are ignored, and the PageRank is just the uniform distribution $I(Q) = 1/N$.

If $F = \epsilon$ for small ϵ (specifically $1/\epsilon$ is much larger than the number of inlinks of any page) then the all pages have PageRank closed to $1/N$. In this case
$I(P) = (1/N)(1 + \epsilon \sum_{Q \to P} 1/O(Q)) + O(\epsilon^2/N)$.

If $F = 1$, the method blows up. There still exists a stationary distribution, but there may be more than one, and iterative algorithms may not converge to any stationary distribution.

If F is close to 1, the system is unstable (i.e. small changes to structure may make large changes to the solution.) The iterative algorithms converge only slowly.

The experiments used in the original PageRank paper used $F = 0.85$.

10.2.2 Pages with no outlinks

Of course, in the actual web, many pages (in fact, the majority of pages — again, a Zipf distribution) have no outlinks. In that case, the above formulas break down, because the denominator $O(P)$ is equal to zero. A number of solutions have been proposed, including the following:

Solution 1: The simplest solution is to add a self-loop from each page to itself. Thus, every page has at least one out-link. The problem is that this rewards a page for not having any out-links. In our random model, if the random browser finds himself at a page with no outlink, he flips the coin until it comes up tails, at which point he jumps at random. With $F = 0.85$, this means that once he reaches a page, he will generally stay there through about 6 more, so a page with no outlinks will be ranked as about 7 times as important as another page with the same real inlinks but many outlinks.

Solution 2: The original PageRank paper proposes the following method:

Step 1: Prune all pages with no outlinks, then prune all pages which had only onlinks to the pages you just pruned, and keep on doing this until all pages have an outlink.
Step 2: Compute PageRank over this set;
Step 3: Reinstate the pages you pruned and let importance propagate, using equation 10.1.

Solution 3: The rank computed in solution 2 seems rather arbitrary. Langville and Meyer (2006) propose a method with a more principled formulation. When the random browser comes to a page with no outlinks, he should simply skip flipping the control coin, and just jump randomly to any page in the web. That seems logical. Equation 10.1 is still satisfied; E is the probability that a non-link based jump from somewhere in the web reaches page P. The stochastic matrix becomes more complicated, because it now contains three kinds of values:

- $M[P, Q] = 1/N$ if Q has no outlinks.
- $M[P, Q] = (1 - F)/N$ if Q has some outlinks, but not to P.
- $M[P, Q] = (1 - F)/N + F/O(Q)$ if Q links to P.

Further, more complex, methods of dealing with "dangling nodes" are studied in Langville and Meyer.

10.2.3 Non-uniform variants

It is not necessary for the "inherent" importance of all pages P to be the same value E; one can have any distribution $E(P)$, representing some other evaluation of inherant importance. For example, one could have $E(P)$ ranked higher for pages on a .edu site, or for the Yahoo home page, or for your own page, etc. Just change E to $E(P)$ in the equations above.

Likewise there may be a reason to think that some outlinks are better than others (e.g. font, font size, links to a different domain are more important than links within a domain.) You can assign $W(Q, P)$ be the weight of the link from Q to P however you want; the only constraints are that the weights are non-negative and that the weights of the outlinks out of Q add up to 1. Replace $1/O_Q$ by $W(Q, P)$ in the equations above.

10.3 Hidden Markov models and the k-gram model

A number of problems in natural language analysis can be formulated in the following terms: You are given a *text*, which is viewed as a string of *elements*. The problem is to assign one *tag* out of a collection of tags to each of the elements. Examples:

- The elements are words, and the tags are parts of speech. In applications, "part of speech" here often involves finer distinctions than the usual linguistic categories. For instance the "named entity" recognition problem involves categorizing proper nouns as personal names, organizations, place names, etc.
- The elements are words and the tags are the meanings of the words (lexical disambiguation).
- The elements are phonemes, as analyzed in a recording of speech, and the tags are words.

In the statistical, or supervised learning, approach to this problem, you are given a large *training corpus* of correctly tagged text. The objective, then, is to extract patterns from the training corpus that can be applied to label the new text.

The same kind of analysis applies in other domains besides natural language analysis. For example, a computer system may be trying to analyse the development over time of some kind of process, based on a sequence of observations that partially characterize the state. Here the elements are the observations and the tags are the underlying state.

10.3.1 The probabilistic model

In a probabilistic model of tagging, we formulate the problem as looking for the *most likely* sequence of tags for the given sequence of elements. Formally, let n be the number of elements in the sentence to be tagged. Let E_i be the random variable for the ith element, let T_i be the random variable for the ith tag, let e_i be the actual value of the ith element. The problem is to find the sequence of tag values $t_1 \dots t_N$ such that $P(T_1 = t_1 \dots T_n = t_n \mid E_1 = e_1 \dots E_N = e_n)$ is as large as possible. We will abbreviate the event $T_i = t_i$ as $\bar{t}_i$ and $E_i = e_i$ as $\bar{e}_i$.

For instance, in tagging the sentence "I can fish", by part of speech we want to arrive somehow at the estimate that $P(T_1$=pronoun,T_2=modal,T_3=verb $\mid$ E_1="I", E_2 ="can", E_2 ="fish $\rangle)$ is large, that $P(T_1$=pronoun,T_2=verb,T_3=noun $\mid$ E_1="I", E_2 ="can", E_2 ="fish" $\rangle)$ (meaning "I put fish into cans") is small and that the probability for any other sequence of three tags is tiny or zero.

In principle, what we're after is this; if you consider all the times that the sentence "I can fish" might be written or spoken, what fraction of the time is the intended meaning the one corresponding to ⟨pronoun modal verb⟩ and what fraction of the time is it the one corresponding to ⟨pronoun verb noun⟩? However, there is obviously no way to directly measure this for most sentences. So we have to estimate this probability in terms of numbers that can actually be measured in a training corpus. As throughout applied probability, to do this we make independence assumptions that are violently and obviously false.

We proceed as follows: We first apply Bayes' Law to derive

$$P(\bar{t}_1 \dots \bar{t}_n \mid \bar{e}_1 \dots \bar{e}_n) = P(\bar{e}_1 \dots \bar{e}_n \mid \bar{t}_1 \dots \bar{t}_n) \cdot P(\bar{t}_1 \dots \bar{t}_n)/P(\bar{e}_1 \dots \bar{e}_n)$$

However the denominator above $P(\bar{e}_1 \dots \bar{e}_n)$ is just a normalizing factor, which only depends on the sequence of elements, which is given. As this is the same for all choices of tags, we can ignore it in comparing one sequence of tags to another.

So we've re-expressed the problem as finding the sequence of tags that maximizes the product $P(\bar{t}_1 \ldots \bar{t}_n) \cdot P(\bar{e}_1 \ldots \bar{e}_n \mid \bar{t}_1 \ldots \bar{t}_n)$ The first factor here is the inherent likelihood of the sequence of tags, before we have seen what the elements are. The second is the likelihood that a particular sequence of tags $\langle t_1 \ldots t_n \rangle$ will be instantiated as the sequence of elements $\langle e_1 \ldots e_n \rangle$. For instance, in the speech understanding problem, the first term is the probability that a speaker will speak a given sentence, sometimes called the "linguistic" model; the second is the probability, given the sentence, that he would pronounce it in the way that has been heard, sometimes called the "phonetic" model. (The interpretation of this product in the "part-of-speech" problem is not as natural.) We now have to estimate these two terms using independence assumptions.

We can use the rule for the probability of a conjunction to expand the second term as follows:

$$P(\bar{e}_1 \ldots \bar{e}_n \mid \bar{t}_1 \ldots \bar{t}_n) = P(\bar{e}_1 \mid \bar{t}_1 \ldots \bar{t}_n) \cdot P(\bar{e}_2 \mid \bar{e}_1, \bar{t}_1 \ldots \bar{t}_n) \cdot \ldots \cdot P(\bar{e}_n \mid \bar{e}_1 \ldots \bar{e}_{n-1}, \bar{t}_1 \ldots \bar{t}_n)$$

We now make the independence assumption that $\bar{e}_i$ depends only on $\bar{t}_i$; specifically, that $\bar{e}_i$ is conditionally independent of $\bar{t}_j$ for $j \neq i$ and of $\bar{e}_j$ for $j < i$. We also make the "time invariance" assumption that the probability that, for example, "pronoun" is instantiated as "he" is the same whether we are talking about the first word in the sentence or about the fifth.[5]

Having made this assumption, we can rewrite the above product in the form $P(\bar{e}_1|\bar{t}_1) \cdot P(\bar{e}_2|\bar{t}_2) \cdot \ldots \cdot P(\bar{e}_n|\bar{t}_n)$. We can now use Bayes' law again, and write this in the form $P(\bar{e}_i|\bar{t}_i) = P(\bar{t}_i|\bar{e}_i)P(\bar{e}_i)/P(\bar{t}_i)$. But again, the factors $P(\bar{e}_i)$ do not depend on under the choice of $\bar{t}_i$, and so can be ignored.

(What is gained by this second turning around? After all whether we use $P(\bar{e}_i|\bar{t}_i)$ or $P(\bar{t}_i \mid \bar{e}_i)/P(\bar{t}_i)$, we will end up estimating it, for each element, in terms of the fraction of instances of t_i in the corpus that are also instances of e_i. The answer is that, since $P(\bar{t}_i \mid \bar{e}_i)$ is the more natural quantity, there may be other sources of information that give good evidence about this, but not about $P(\bar{e}_i|\bar{t}_i)$. For instance, we may have a dictionary, which shows a word has possible parts of speech that do not appear in the training corpus. In that case, we can assign $P(\bar{t}_i \mid \bar{e}_i)$ some default estimate on the strength of the dictionary entry.)

We now turn to the first term in the original product above: $P(\bar{t}_1 \ldots \bar{t}_n)$. Again using the rule for conjunctions, we can write this in the form,

$$P(\bar{t}_1 \ldots \bar{t}_n) = P(\bar{t}_1) \cdot P(\bar{t}_2 \mid \bar{t}_1) \cdot P(\bar{t}_3 \mid \bar{t}_1, \bar{t}_2) \cdot \ldots \cdot P(\bar{t}_n \mid \bar{t}_1 \ldots \bar{t}_{n-1}).$$

We now make the second independence assumption, known as the k-gram assumption, for some small integer k: the dependence of the ith tag on all the previous tags in fact reduces to its dependence on the $k-1$ previous tags. More precisely stated, T_i is conditionally independent of $T_1 \ldots T_{i-k}$ given $T_{i+1-k} \ldots T_{i-1}$. Thus $P(\bar{t}_i \mid \bar{t}_1 \ldots \bar{t}_{i-1}) = P(\bar{t}_i \mid \bar{t}_{i+1-k} \ldots \bar{t}_{i-1})$.

From this point forward in this section, to simplify the notation, we will consider the case $k = 3$, which is the most commonly used value; however, it should be easy to see how the formulas below can be modified for other values of k. The trigram assumption ($k = 3$) states that T_i is conditionally independent of $T_1 \ldots T_{i-3}$ given T_{i-2}, T_{i-1}. Thus $P(\bar{t}_i \mid \bar{t}_1 \ldots \bar{t}_{i-1}) = P(\bar{t}_i \mid \bar{t}_{i-2}, \bar{t}_{i-1})$.
Again we make the time invariance assumption, that this probability is the same for all values of $i > k$.

In order to get a more uniform notation, we make the convention that there are two random variables T_{-1} and T_0 that have the special tag *S* (start) with probability 1. We can then write the above product in the form $P(\bar{t}_1 \ldots \bar{t}_n) = \Pi_{i=1}^{n} P(\bar{t}_i|\bar{t}_{i-2}, \bar{t}_{i-1})$

[5]To express this condition mathematically would require making our notation substantially more complicated. This is common in write-ups of complex probabilistic models like this; substantial parts of the theory are left either stated only in English, or left entirely implicit, to be understood by the reader.

Putting all this together we get the formula

$$P(\bar{t}_1 \ldots \bar{t}_n \mid \bar{e}_1 \ldots \bar{e}_n) = \alpha \cdot \Pi_{i=1}^{n} \frac{P(\bar{t}_i|\bar{e}_i) \cdot P(\bar{t}_i|\bar{t}_{i-2}, \bar{t}_{i-1})}{P(\bar{t}_i)}$$

10.3.2 Hidden Markov models

Based these independence assumptions, we can now view sentences as the output of the following random process. The process outputs a sequence of ⟨tag,element⟩ pairs. The *state* is the pair $\langle t_{i-2}, t_{i-1}\rangle$ of the last two tags that it has output (in the general k-gram model, this is the tuple of the last $k-1$ tags it has output.) If the process is in state $\langle t_{i-2}, t_{i-1}\rangle$, then it first picks a new tag t_i to output, with probability distribution $P(\bar{t}_i|\bar{t}_{i-2}, \bar{t}_{i-1})$ and then based on that tag, picks an element e_i with probability distribution $P(\bar{e}_i|\bar{t}_i)$. The new state is $\langle t_{i-1}, t_i\rangle$. The problem we have to solve is that we are given the sequence of elements $\langle e_1 \ldots e_n\rangle$ and we wish to find the sequence of tags $\langle t_1 \ldots t_n\rangle$ for which the posterior probability $P(\bar{t}_1 \ldots \bar{t}_n \,|\, \bar{e}_1 \ldots \bar{e}_n)$ is maximal. Note that finding the sequence of states is equivalent to finding the sequence of tags; if the process goes from state $\langle x, y\rangle$ to $\langle y, z\rangle$ then the tag output is z.

This is an instance of a *hidden Markov Model (HMM)*. A hidden Markov model is a modified Markov model in which:

- There is a particular starting state s_0.
- There may be multiple arcs between any two vertices. (For that reason, the transition matrix representation cannot be used.)
- Each arc is labelled by an element.
- The arc $A(u, e, v)$ from state u to state v labelled e is labelled by the probability $P(A(u, e, v)|u)$, the probability, given that you are in state u at time t, that you will proceed to traverse arc $A(u, e, v)$. These probabilities on the outarcs from u form a probability distribution.

As the process moves on a path through the model, it outputs the elements that label the arcs it traverses. The problem is, given a sequence of output elements, what is the most probable path that outputs that sequence? The model is called "hidden" because all we see is the sequence of elements, not the sequence of states.

To solve this, we proceed as follows:

$$P(S_0 = s_0, S_1 = s_2 \ldots S_n = s_n \mid S_0 = s_0, \bar{e}_1 \ldots \bar{e}_n) =$$

$$\frac{P(S_0 = s_0, \bar{e}_1, S_1 = s_1, \bar{e}_2, S_2 = s_2, \ldots S_n = s_n, \bar{e}_n, S_{n+1} = s_{n+1} \mid S_0 = s_0)}{P(\bar{e}_1 \ldots \bar{e}_n)} =$$

$$\alpha \cdot \Pi_{i=1}^{n} P(A(s_{i-1}, e_i, s_i) \mid s_{i-1})$$

where α is a normalizing factor depending only on the e_i and not on the s_i.

In the case of the k-gram model, as we have seen,

$$P(A(\langle t_{i-2}, t_{i-1}\rangle,\ e_i,\ \langle t_{i-1}, t_i\rangle)) = \alpha \frac{P(\bar{t}_i \mid \bar{e}_i) \cdot P(\bar{t}_i \mid t_{i-2}, t_{i-1})}{P(\bar{t}_i)}$$

For convenience in computation, we use the negative logarithm of the probability of the path; maximizing the probability is equivalent to minimizing the negative logarithm. This both replaces

maximizing a product by minimizing a sum, which is a more standard formulation, and avoids the risk of underflow. Discarding the normalization factor α, which does not affect the choice of maximum, our task is now to maximize the expression,

$$-\log_2(\Pi_{i=1}^{n}\frac{P(\bar{t}_i|\bar{e}_i)\cdot P(\bar{t}_i|\bar{t}_{i-2},\bar{t}_{i-1})}{P(\bar{t}_i)}) = \sum_{i=1}^{n} -\log_2(\frac{P(\bar{t}_i|\bar{e}_i)\cdot P(\bar{t}_i|\bar{t}_{i-2},\bar{t}_{i-1})}{P(\bar{t}_i)})$$

10.3.3 The Viterbi algorithm

In our analysis above, we have reduced the problem of finding the most probable sequence of tags to the following graph algorithm problem:

> Given:
>
> 1. A directed multi-graph M (i.e. a graph with multiple arcs between vertices), where each arc is labelled with an element and a numeric weight.
>
> 2. A particular starting vertex $S0$ in M.
>
> 2. A string W of N elements.
>
> To find: The path through M that traverses arcs labelled with the elements in S in sequence such that the sum of the weights is maximal.

Since there are, in general, exponentially many such paths, one might naively suppose that the problem is intractable. In fact, however, it is easily reduced to the well-known single-source shortest-paths graph problem. Construct a graph G as follows:

- The vertices in G are all pairs $\langle V, I\rangle$ where V is a vertex of M and I is an integer from 1 to N, plus a final vertex END.
- There is an edge from $\langle U, I-1\rangle$ to $\langle V, I\rangle$ in G just if there is an edge from U to V in M whose label is $S[I]$.
- There is an edge of weight 0 from every vertex $\langle V, N\rangle$ to END.

Clearly, any path through M starting in $S0$ that outputs W corresponds to a path through G from $\langle S0, 0\rangle$ to END.

Because the graph G is "layered" — that is, all arcs go from a vertex in the Ith layer to one in the $I+1$st layer — the algorithm to solve this is particularly simple. The cost of the shortest path ending at a vertex V in layer $I+1$ is the minimum over all vertices U in layer I of [the cost of the shortest path to U plus the cost of the arc from U to V]. Details of the algorithm, known as "Viterbi's algorithm", are given in table 10.1, and an example is given in section 10.3.4. There are some easy further optimizations that can be carried out. In particular, as you generate states at the Ith level, you check that they have an outarc labelled $W[I]$ and you put them on a list; that way, on the next iteration you can just go through the list of states that satisfy the two tests, "$E = W[I]$ and $Total[U, I-1] \neq \infty$", which may be much smaller than the set of all states. Also, once all the values of $Total$ at level $I+1$ have been calculated, the values at level I can be overwritten, saving some space.

10.3.4 Example: Part of speech tagging

Consider the following toy example:

```
function Viterbi
      (in W : string of elements of length N;
          M = ⟨SS, AA⟩ : directed multigraph.
                Each arc A in AA has the form ⟨ tail, element, head ⟩;
          C(A); numerical cost of arcs in AA;
          S0: starting state in M)
      return path of minimal total cost through M starting in S0 and outputting W;

/* The array Total(S, I) is the total cost of the shortest path through M from S0 to S
      traversing the first I elements of W.
The array Back(S, I) is the state preceding S on this path.
The graph G discussed in the text is left implicit, rather than constructed explicitly. */

{ Construct arrays Total(S, I) and Back(S, I) where S ∈ SS and I ∈ 0 ... N;
  Initialize Total to ∞;
  Total[S0, 0] = 0;

  for (I ← 1 ... N) {
      for (each arc A = ⟨U, E, V⟩) in AA {
          if (E = W[I] and Total[U, I − 1] ≠ ∞) {
            NewWeight ← Total[U, I − 1] + C(A);
            if NewWeight < Total(V, I) {
              Total(V, I) ← NewWeight;
              Back(V, I) ← U;
            } } } }

/* Find the best path by tracing back pointers from the best final state. */
  Best ← the state S for which Total(S, N) is minimal;
  Path ← ⟨Best⟩;
  for (I ← N ... 1) {
      Best ← Back(Best, I);
      Path ← Best, Path;
      }

return Path;
}
```

Table 10.1: Viterbi algorithm

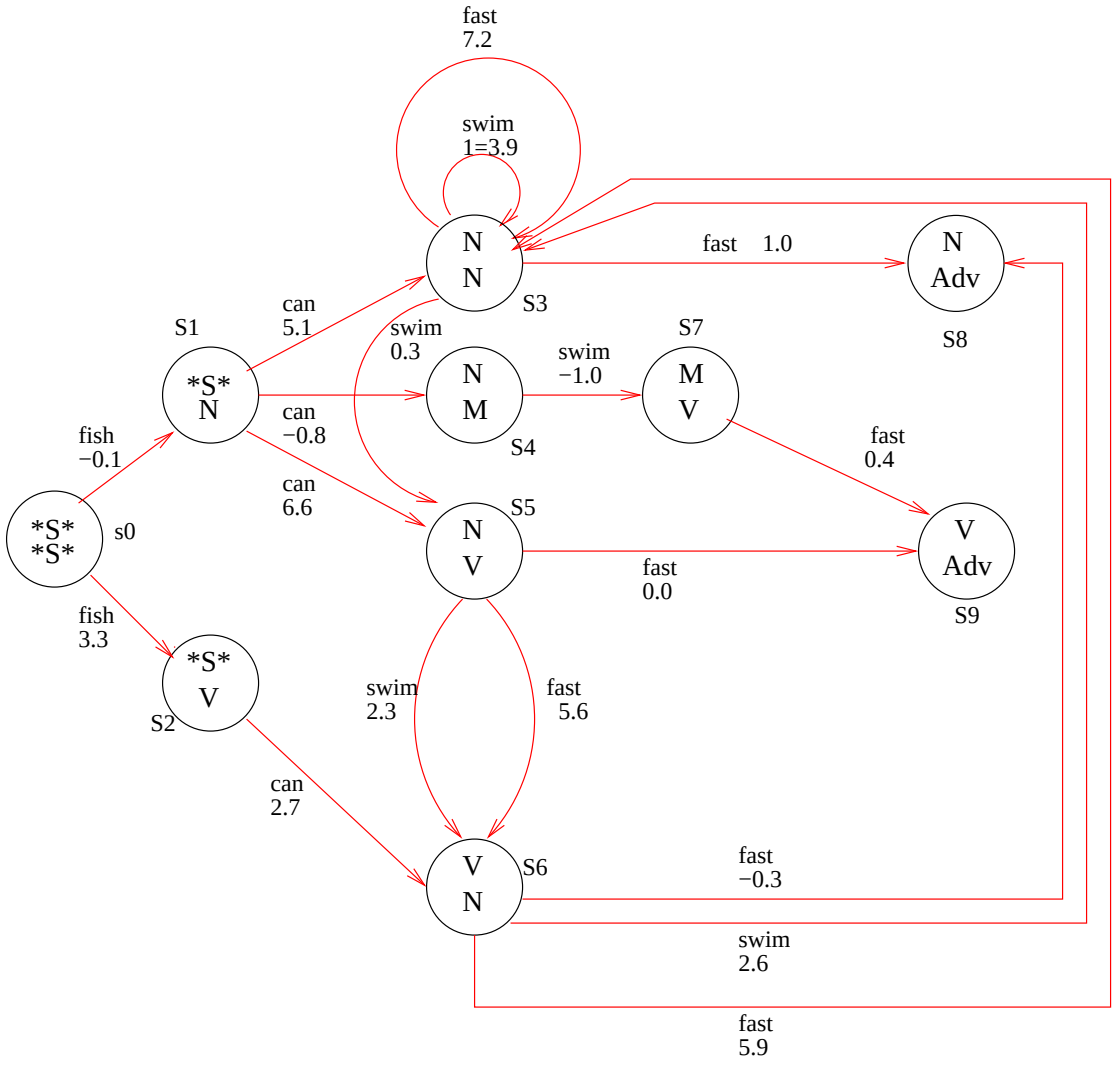


Figure 10.4: Markov model for part of speech tagging

Fish can swim fast.

Note that:

- "Fish" and "swim" can be nouns or verbs (go fishing).
- "Can" can be a modal, a noun, or a verb (pack stuff into cans)
- "Fast" can be an adverb ("he works fast"), an adjective ("a fast horse"), a noun ("the fast of Yom Kippur") or a verb ("Jews fast on Yom Kippur"). However, to simplify this example, we will consider only the possibilities adverb and noun.

We will use a trigram model, and we will suppose that we have the following probabilities shown in table 10.2.

Figure 10.4 shows the corresponding Markov model. The weights on an arc from state $\langle t1, t_2 \rangle$ to $\langle t_2, t_3 \rangle$ labelled e is equal to $-\log_2(\frac{P(\bar{e}_i|\bar{t}_i) \cdot P(\bar{t}_i|\bar{t}_{i+1-k}, \bar{t}_{i-1})}{P(\bar{t}_i)})$

Only the probabilities relevant to the sample sentence are shown. Probabilities not shown are either zero or are irrelevant (i.e. appear only in terms where they are multiplied by zero).

Relevant absolute tag probabilities:

P(N) = 0.3
P(V) = 0.2
P(M) = 0.1
P(Adv) = 0.1

Tag given element probabilities:

P(N |"fish") = 0.8
P(V |"fish") = 0.2
P(M |"can") = 0.9
P(N |"can") = 0.09
P(V |"can") = 0.01
P(N |"swim") = 0.2
P(V |"swim") = 0.8
P(Adv |"fast") = 0.5
P(N | "fast") = 0.02

Relevant Transitional Probabilities

P(N | *S* *S*) = 0.4
P(V | *S* *S*) = 0.1
P(M | *S* N) = 0.2
P(V | *S* N) = 0.2
P(N | *S* N) = 0.1
P(N | *S* V) = 0.5
P(N | M V) = 0.35
P(Adv | M V) = 0.15
P(V | N M) = 0.5.
P(M | N N) = 0.2
P(V | N N) = 0.2
P(N | N N) = 0.1
P(Adv | N N) = 0.1
P(N | N V) = 0.3
P(Adv | N V) = 0.2
P(N | V N) = 0.25
P(Adv | V N) = 0.25

Table 10.2: Example: Part of speech tagging

Infinite values are not shown.

At the start

Total(S0,0) = 0.

After 1 word

Total(S1,1) = Total(S0.0) + C(S0, "fish", S1) =	−0.1.	Back(S1,1) = S0
Total(S2,1) = Total(S0.0) + C(S0, "fish", S2) =	3.3.	Back(S2,1) = S0

After 2 words

Total(S3,2) = Total(S1,1) + C(S1, "can", S3) =	5.0.	Back(S3,2) = S1
Total(S4,2) = Total(S1,1) + C(S1, "can", S4) =	−0.9.	Back(S4,2) = S1
Total(S5,2) = Total(S1,1) + C(S1, "can", S5) =	6.5.	Back(S5,2) = S1
Total(S6,2) = Total(S2,1) + C(S2, "can", S6) =	6.0.	Back(S6,2) = S2

After 3 words

Total(S3.3) = min(Total(S3.2) + C(S3, "swim", S3), Total(S6.2) + C(S6, "swim", S3)) =	8.6	Back(S3,3) = S6
Total(S5,3) = Total(S3,2) + C(S3, "swim", S5) =	5.3.	Back(S5,3) = S3
Total(S6,3) = Total(S5,2) + C(S5, "swim", S6) =	8.8.	Back(S6,3) = S5
Total(S7,3) = Total(S4,2) + C(S4, "swim", S7) =	−1.9	Back(S7,3) = S4

After 4 words

Total(S3,4) = min(Total(S3,3) + C(S3, "fast", S3), Total(S6,3) + C(S6, "fast", S3)) =	14.7.	Back(S3,4) = S6
Total(S6,4) = Total(S5,3) + C(S5, fast", S6) =	10.9.	Back(S6,4) = S5
Total(S8,4) = min(Total(S3,3) + C(S3, "fast", S8), Total(S6,3) + C(S6, "fast", S8)) =	8.5.	Back(S3,4) = S6
Total(S9,4) = min(Total(S7,3) + C(S7, "fast", S9), Total(S5,3) + C(S5, "fast", S9)) =	−1.5.	Back(S9,4) = S7

Table 10.3: Execution of Viterbi's algorithm

For example, the arc labelled "can" from state S1 to S4 has weight

$$-\log_2(P(\text{M} \mid \text{"can"}) \cdot P(M \mid SN)/P(M)) = -\log_2(0.9 \cdot 0.4/0.1) = -1.8480$$

The numbers on the arcs in figure 10.4 are negative logs of unnormalized probabilities; and thus their interpretation is a little abstruse. If we consider the probability that a given arc will be traversed, given the starting state and the element, for two different arcs, then the ratio of those probabilities is is 2^{L2-L1} where $L1$ and $L2$ are the two labels. For example, the arc labelled "swim" from $S4$ to $S7$ is -1.0 the arc labelled "can" from $S2$ to $S6$ is 2.7. Therefore

$$P(T_3 = V|T_1 = N, T_2 = M, E_3 = \text{“}swim''')/P(T_2 = N|T_0 = *S*, T_1 = V, E_2 = \text{“}can'') = 2^{3.7} = 13.$$

The execution of Viterbi's algorithm proceeds as in table 10.3.

The result of table 10.3 is that S9 is the winning state with a score of -1.5. Tracing backward from S9 the winning tagging found to be is ⟨ N, M, V, Adv ⟩, as one would expect.

10.3.5 The sparse data problem and smoothing

To compute the above product, we need three types of probabilities: $P(t_i|t_{i+1-k}\ldots t_{i-1})$, $P(t_i|e_i)$ and $P(t_i)$ This is where our training corpus comes in: We estimate each of these quantities by the frequency in the corpus:

$P(t_i|t_{i-2}, t_{i-1}) = \text{Freq}_C(t_i|t_{i-2}, t_{i-1})$.
$P(t_i|e_i) = \text{Freq}_C(t_i|e_i)$.
$P(t_i) = \text{Freq}_C(t_i)$.

where $\text{Freq}_C(\cdot)$ means the frequency in the training corpus C.

Unfortunately, there is often a problem with the first of these in particular; namely, that some possible k-tuples of tags $t_{i+1-k}\ldots t_i$ may actually never occur in the corpus C. This is unlikely in the case where the tags are parts of speech, but is altogether likely in the case where the tags are words. (As discussed in section 9.6.3, the frequency of trigrams in text follows a Zipf distribution with a very long tail.)

We have seen this kind of problem before, with Naive Bayes classifiers (section 8.11) and the solution we use here is a similar kind of smoothing. We estimate the probability of the k-gram as a weighted sum of the unigram, the bigram, the trigram, ... the $k-1$ gram. For example, with $k = 3$ we estimate

$$P(\bar{t}_i|\bar{t}_{i-2}, \bar{t}_{i-1}) = \alpha_1 \underset{C}{\text{Freq}}(\bar{t}_i|\bar{t}_{i-2}, \bar{t}_{i-1}) + \alpha_2 \underset{C}{\text{Freq}}(\bar{t}_i|\bar{t}_{i-1}) + \alpha_3 \underset{C}{\text{Freq}}(\bar{t}_i)$$

where $\alpha_1, \alpha_2, \alpha_3$ are weights (e.g. 0.6, 0.3, 0.1). For instance, we estimate the probability of seeing "jelly" following "burnt strawberry" as 0.7 times the frequency with which "burnt strawberry" is followed by "jelly" in the corpus, plus 0.2 times the frequency with which "strawberry" is followed by "jelly" in the corpus, plus 0.1 times the frequency of "jelly" in the corpus. Thus, we give preference to trigrams that actually occur in the corpus, while admitting the possibility of seeing new trigrams and even new bigrams.

Exercises

Use MATLAB for all these exercises.

Exercise 10.1

Consider the Markov model shown in figure 10.5

A. What is the transition matrix for the model?

B. Assume that at time 0 the probability of state A is 1. What is the probability distribution at time 1? At time 2? At time 10?

C. What is the stationary probability distribution for the model?

Exercise 10.2

(Time consuming, but possibly fun): Construct the Markov model for a player's position at the end of each roll of the dice on the standard Monopoly board, keeping in mind (a) that if you land on "Go

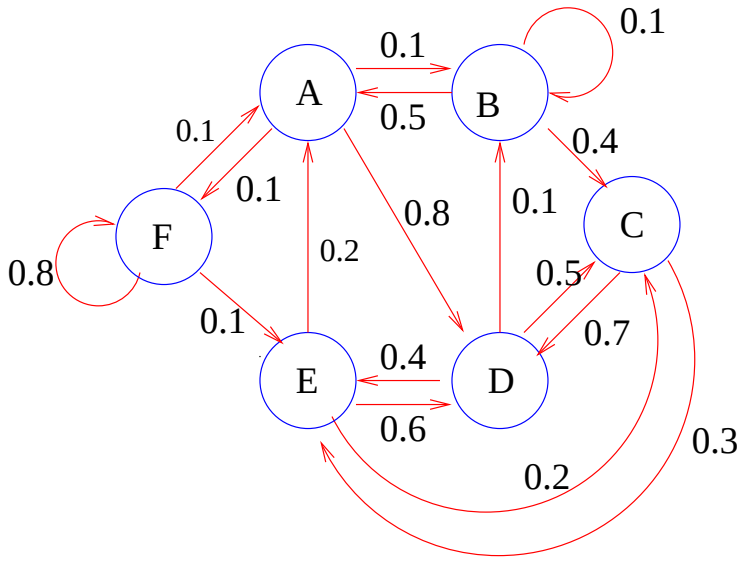


Figure 10.5: Markov model for Exercise 10.1

to jail" you go to jail; (b) that if you land on Community Chest or Chance, with some probability you will get a card sending you somewhere else (nearest railroad, St. Mark's Place, Go, etc.). Ignore the rule that you go to jail if you roll three doubles in a row, and assume that the player always pays to get out of jail. Use MATLAB to compute the stationary distribution for the model. Can you glean any useful strategic hints?

Exercise 10.3

A. Redo the PageRank computation on page 266 using $F = 0.1$, $E = 0.15$. How do the new results compare to the old ones? Give an intuitive explanation.

B. Modify the graph in figure 10.3 by adding arcs from U to W and from W to U. Compute the PageRank in the new graph, using $F = 0.7, e = 0.05$. How does the results compare to the PageRank in the original graph? Give an intuitive explanation.

Exercise 10.4

Compute the absolute probabilities of all the possible taggings of the sentence "Fish can swim fast", using the model in section 10.3.4.

Problems

Problem 10.1

The *one-dimensional random walk with absorption* is the following Markov model:

- There are $2N + 1$ states, labelled $-N, \ldots -1, 0, 1, N$.

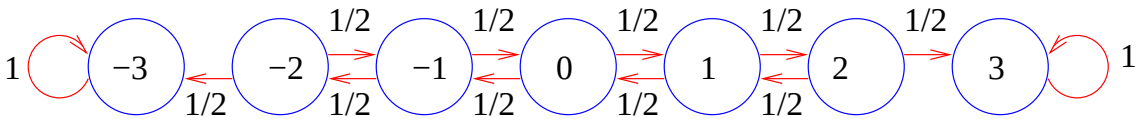


Figure 10.6: Random walk with N=3

- If $K \neq -N, N$ then there are two transitions from K, one to $K-1$ and one to $K+1$, each with probability $1/2$.
- The only transition from N and from $-N$ is to itself with probability 1.

Figure 10.6 illustrates the model with $N = 3$.

A. There is more than one stationary distribution for the random walk. Characterize the space of stationary distributions. (You should be able to solve this problem without using MATLAB.)

B. Generate the transition matrix for the case $N = 50$.

C. Let $N = 50$. Assume that at time 0 the system is in state 0 with probability 1. Compute the distribution at time 50. Plot the distribution. What does it look like? Explain this outcome.

D. Let $N = 50$. Clearly any random walker will either find his way to state 50 or to state -50 and then will stay there forever. We can define a function $f(I)$ which is the probability that a walker will end up in state 50 given that at some earlier time he is at state I. The value $f(-50) \ldots f(0) \ldots f(50)$ satisfy a system of linear equations. Describe the system of linear equations, and solve them, either using MATLAB or by inspection.

Problem 10.2

Suppose that a Markov model has two different stationary distributions $\vec{p}$ and $\vec{q}$. Show that, for any t such that $0 < t < 1$, $t \cdot \vec{p} + (1-t)\vec{q}$ is also a stationary distribution. Note that there are two things you have to show: first, that this is stationary and second, that it is a legitimate distribution.

Problem 10.3

Construct an example of a Markov model which has only one stationary distribution, but where there are starting distributions that do not converge to the stationary distribution. (Hint: There is an example with only two states.)

Programming Assignments

Assignment 10.1

A. Write a function `PageRank(A,E)` that computes page rank based on links, as described in the class notes. The input parameter A is an $N \times N$ adjacency matrix; $A(I, J) = 1$ if page I has a link to page J. The input parameter E corresponds to the probabilistic parameter e as described in the notes.

Ignore any self-loops. Treat a page with no outlinks as if it had an outlink to every other page, as in solution 3, section 10.2.2 of the notes.

B. Choose some specific collection of interlinked documents; e.g. the Wikipedia pages for U.S. Presidents, or some collection of messages on a chat board. Construct the link graph between the documents, and compute the PageRank. Order the documents by PageRank. Does the ordering correspond well to your own sense of the relative importance of these documents?

Chapter 11

Confidence Intervals

11.1 The basic formula for confidence intervals

Suppose that you carry out a poll of 1000 randomly chosen Americans, asking each of them whether they prefer apple pie or blueberry pie. 574 prefers apple; 426 prefers blueberry. What can you say about the fraction of the entire population that prefers apple pie? It would not be reasonable to conclude with certainty that exactly 57.4% of the population prefers apple. On the other hand, it seems safe to conclude with near certainty that the true fraction is larger than 10% and smaller than 90%. What you would like to assert, clearly, is a statement of the form, "The fraction of the population that prefers apple pie is probably somewhere close to 57.4%", with some numbers attached to the vague terms "probably" and "somewhere close"; for example "the probability is at least 95% that the fraction of people who prefer apple pie is between 54% and 60%." Symbolically, let f be the true fraction of the population and let $\bar{f} = 0.574$ be the fraction in the poll. Then the claim is $P(0.54 \leq f \leq 0.60 \mid \bar{f} = 0.574) \geq 0.95$. The interval $[0.54, 0.60]$ is called the *confidence interval for f at the 95% level*. (Sometimes it is called the confidence interval at the 5% level. Since no one is ever interested in intervals where the probability is less than 1/2, this does not give rise to ambiguity.)

The actual calculation is quite simple, but the justification is complicated. In fact, the same calculation can be justified in two quite different ways, one corresponding to the likelihood theory of probability and one corresponding to the frequentist theory. Since 99% of the time, all you need is to do the calculation (and 99% of the people who do these calculations neither understand the justification nor care about it) we will begin here how to do the calculation, and we will point out some important features of it. The justifications will be discussed in optional sections 11.3 and 11.4.

Here is the formula. As long as the sample size n is large, the sample fraction $\bar{f}$ is not close to 0 or to 1, and you are not interested in probabilities *very* close to 1 (that is, probabilities like $1 - 2^{-n}$), then you can consider that the true fraction f follows a Gaussian distribution, whose mean is $\bar{f}$ and whose standard deviation is $\sigma = \sqrt{\bar{f}(1-\bar{f})/n}$. Specifically, let $E(x)$ be the integral of the standard Gaussian: $E(x) = \int_{-\infty}^{x} N_{0,1}(t)dt$. For any q which is substantially less than $\min(f, 1-f)/\sigma$, the probability that f lies within $q \cdot \sigma$ of $\bar{f}$ is

$$P(\bar{f} - q \cdot \sigma \leq f \leq \bar{f} + q \cdot \sigma) = \int_{\bar{f}-q\cdot\sigma}^{\bar{f}+q\cdot\sigma} N_{\bar{f},\sigma}(t)dt = \int_{-q}^{q} N_{0,1}(x)dx = 2E(q) - 1$$

Therefore, to get a confidence interval at level p, look up $E^{-1}((p+1)/2)$ in a table, or compute the

MATLAB expression `erfinv(p)*sqrt(2)` (see section 9.9) and that is the value of q. The confidence interval at level p is then $[\bar{f} - q \cdot \sigma, \bar{f} + q \cdot \sigma]$.

For example, suppose we have the above poll, with $n = 1000$ and $\bar{f} = 0.574$, and we want to get a confidence interval at the 95% level. We compute $\sigma = \sqrt{\bar{f}(1-\bar{f})/n} = 0.0156$. We have $(1 + p)/2 = .975$ and we can find out that $q = E^{-1}(0.975) = 1.96$. Therefore the 95% confidence interval is

$$[0.574 - 1.96 \cdot 0.0156,\ 0.574 + 1.96 \cdot 0.0156] = [0.5434, 0.6046].$$

This is the "±3% margin of error" that is always reported together with political polls.

If you want to do a back-of-the envelope estimate, and you don't have the inverse Gaussian integral handy, you can do as follows: First, $\sqrt{\bar{f}(1-\bar{f})}$ is pretty much 1/2 for most reasonable values of $\bar{f}$; if $\bar{f}$ is between 0.2 and 0.8 then $\sqrt{\bar{f}(1-\bar{f})}$ is between 0.4 and 0.5. So σ is pretty much $1/2\sqrt{n}$. Second, you really only need to remember 3 values of q:

A 5% confidence interval is 2 standard deviations.
A 1% confidence interval is 2.6 standard deviations.
A 0.1% confidence interval is 3.3 standard deviations.

So as long as you know how to estimate $\sqrt{n}$, you're all set.

Four general points about sampling and confidence intervals should be kept in mind.

First, the standard deviation σ is proportional to $1/\sqrt{n}$. Therefore, to reduce the width of the confidence interval by a factor of k, it is necessary to increase the sample size by k^2. That is the reason that every political poll you have ever seen had a sample size of about 1000 and a 3% margin of error. To reduce the margin of error to 1% would require sampling 9000 people, and would therefore cost 9 times as much to carry out; it's not worthwhile, considering that the numbers will be all different next week anyway. (Self-selecting polls, such as Internet votes, can have much higher values of n, but gauging the accuracy of such a poll is a very different question.)

Second, the confidence interval does not at all depend on the size of the population, as long as the population is large enough that one can validly approximate sampling without replacement by sampling with replacement. (If you sample *with* replacement, then the same confidence intervals apply even if the actual population is *smaller* than the sample; that is, you ask everyone the same question several times.) A sample of size 1000 has a ±3% confidence interval at the 95% level, whether the population is ten thousand or ten billion.

Third, you are now in a position to be as annoyed as I always am when you hear a TV pundit, in one sentence, states responsibly that the poll he has quoted has a margin of error of 3%, and in the next sentence, speculate on the reason it went from 55% yesterday to 54% today. For a poll with $n = 1000$ and $\bar{f} = 0.55$, the interval $[0.54, 0.56]$ has confidence 0.495. So there is a better than 50% chance that two polls of 1000 people will differ by 1% in one direction or the other, purely by chance, even if they are conducted in the same way and taken at the same time. There is no need to look for any other reason.

The fourth point is the most important, though it runs the risk of sounding like the villainous lawyers for PG&E in *Erin Brockovich.* If you set your significance level at 99% then, in one out of every 100 experiments, you will get results that pass the test, just due to chance. If you are mining medical data looking for a cause of a disease, and you have records of 1000 different possible influences, then you will probably find 10 that are significant at the 99% level and one that is significant at the 99.9% level, even if they are all actually independent of the disease. If you run a statistical test on your particular city and you find that the incidence of bone cancer is above the national average with a confidence of 99.9%, then you have reason to suspect that there may well be an environmental cause. But if someone in each of the 30,000 cities in the United States runs such a test, then you have to

expect that 30 of these will come up positive, even if there is no environmental cause anywhere. The moral is that you have to be very careful in drawing conclusions purely from statistical evidence.[1]

11.2 Application: Evaluating a classifier

One of the most common uses of confidence intervals in computer science is for evaluating the quality of a classifier. As discussed in section 8.11, a *classifier* is a program that determines whether or not a given instance belongs to a given category; for example, whether an email message is spam. Most classifiers are constructed at least in part by applying a supervised machine learning (ML) techniques to a corpus of lablled examples. Suppose that we have such a classifier; how do we measure how well it works?

First, we must decide on a measure of "goodness". For our discussion here, we will take that to be the *overall accuracy* of the classifier; that is, the fraction of instances that are correctly classified, in either direction.

The standard approach is as follows: We begin by randomly separating the labelled corpus into a *training set* R and a *test set* E, We then use the training set R as input to the ML algorithm A, which outputs a classifier A_R. We run the classifier A_R on the test set E; determine the accuracy of A_R over E; and calculate a confidence interval $[L, U]$ at level p based on the size of E.

We can now make the following claim: Let Ω be the probability space of all instances. Assume that the corpus C is a random sample of Ω; this is a large assumption, which is generally difficult to justify, but generally works out well enough. In that case the test set and the training set are nearly independent[2] random samples of Ω, since they were chosen randomly from the corpus; and therefore the event "Instance I is in E" is independent of the event "A_R labels I correctly" relative to the probability distribution Ω. Therefore, the confidence interval we have calculated is valid.

Why should we not run the ML algorithm on the entire corpus, and then test it on the test set – or, for that matter, test it on the entire corpus? The answer is that, if $R \subset E$ or $R = E$, then A_R is not longer independent of E, because A has used E in computing the classifier. In the extreme case, suppose that the classifier output by A_R consists of a pair: a general rule to be used on examples that are not in R; and a hash table with the answer recorded for all the instances in R.[3]. In that case, if $E \subset R$, then the accuracy of A_R on E will be 1; however, this is no reason to think that this is a good estimate of the accuracy of A_R over Ω.

In practice, of course, machine learning algorithms generally do better the larger the training set; and it seems like a pity to throw away useful training data. Therefore what is often done in practice is that, after the classifier has been evaluated, the learning algorithm is rerun on all the data, and one assumes that the new classifier, based on more data, is at least as good as the classifier that was evaluated. (There are some learning algorithms for which it is possible to prove that, on average, they do better given more data, and some where it is currently just a plausible assumption.)

One issue that requires care relates to the problem of multiple experiments discussed at the end of the previous section. In general, there are many different machine learning techniques that can be used for any given application, and each general technique can be used with a variety of options, parameter settings, feature spaces, and so on. Suppose that you divide the corpus into a training set R and a test set E of size 1000; you run a hundred different machine learning techniques over

[1] This kind of problem has recently become a major concern in scientific research. See for example the article "Why most published research findings are false", (Ioannidis 2005).

[2] They are not quite independent, because they are mutually exclusive.

[3] This may seem like an absurd cheat, but if the distribution over examples follows a power-law, so that a large fraction of the instances encountered come from a small number of cases, it may be perfectly reasonable (section 9.6.3)

```
function CrossValidate(in D: labelled data; M: classification algorithm)
                        return estimate of accuracy

{ Partition the data D into ten subsets S_1 ... S_10;
  for (i ← 1 ... 10)
      R ← D \ S_i;
      C ← M(R); /* Compute classifier */
      A_i ← accuracy of C on S_i;
  endfor
  return average of the A_i.
}
```

Table 11.1: Cross-validation algorithm

R; you evaluate all the output classifiers using E; and you get an accuracy for each one. Let us say that these range from 0.64 to 0.72. You now, naturally, take the classifier that did best — call it "$CBest$" – and you publish a paper that claims that the accuracy of $CBest$ has a confidence interval [0.69,0.75] at the 95% confidence level. This claim, however, is not justified. It is quite possible that the classifiers are all of *equal* quality; they each have a 0.68 chance of being correct on any given item. If the classifiers are independent of one another,[4] then with 100 classifiers, you are likely to get one of accuracy 0.72 just by chance. (It is, however, proper to publish a paper that describes the entire procedure of running 100 classifiers, and in that context, you may certainly say that $CBest$ had an accuracy of 0.72.)

To get a proper evaluation of the classifier, you need a new test set. This test set has to be independent of both R and E set, because both of these have been used in formulating $CBest$; R to train it, and E to select it. Another way of viewing this is that the overall procedure, "Run these 100 ML techniques on R; test them on E; choose the best," is itself a meta-ML procedure that takes $R \cup E$ as input and generates the classifier $CBest$. E cannot be used to evaluate $CBest$ because it was part of the input to the program that generated $CBest$.

Therefore, if a scientist anticipates that he/she will be testing multiple classifiers and choosing the best, and if there is plenty of labelled data, then a common practice is to divide the corpus of data into *three* parts: the training set R, the test set E, and the validation set V. The scientist then trains each of the machine learning algorithms on R; test using V; choose the best $CBest$; and then re-evaluate $CBest$ using the test set E. This evaluation of $CBest$ is valid. However, if this re-evaluation does not produce satisfying results, it is not permissible to go and test the *second-best* on V and see if it does better on E and then publish that, if that seems better; because now the same test set has again been used both for selection and for evaluation.

A very common problem and very difficult problem in evaluating classifiers is that labelled data is often limited and expensive to get. If you have only 100 items of labelled data, then you cannot very well spare 30 of those for testing purposes; and in any case a test set of size 30 has a 95% confidence interval of $\pm 18\%$, which is so large as to be useless. One technique that is often used in this case is *cross-validation*, shown in table 11.1. The data is divided 10 different ways into a training set and a validation set; the classifier is trained on the training set and evaluated on the validation set; and the average accuracy is returned. However, it is difficult to analyze this technique statistically or to determine valid confidence intervals for the result, because the different iterations are anything but independent.

[4] They almost certainly are not, but for the sake of argument.

11.3 Bayesian statistical inference (Optional)

The derivation and interpretation of confidence intervals in the likelihood (Bayesian) interpretation of probability theory is quite straightforward. Let F be a random variable whose value is the fraction of the whole population that prefers apple pie. This is "random" in the sense of likelihood judgement; we don't know what it is, and so there is some chance of it having any value between 0 and 1. If the population count is known to be M, then the value of F must actually have the form i/M, but for simplicity we will approximate this as a continuous probability density. Let X be a random variable where $X = \bar{f}$ is the event that, in a random sample of size n, the fraction that prefers apple pie is $\bar{f}$. What we want to know is the probability distribution of $\tilde{P}(F = t|X = 0.574)$ over all values of t.

As so often, we start with Bayes' law and write

$$\tilde{P}(F = t|X = 0.574) = P(X = 0.574|F = t)\tilde{P}(F = t)/P(X = 0.574)$$

We know how to compute the first expression $P(X = 0.574|F = t)$; this is given by the binomial distribution as $B_{1000,t}(574)$. The denominator is just a constant normalizing factor, independent of t. But what is $\tilde{P}(F = t)$?

$\tilde{P}(F = t)$ is called the *prior;* it expresses your preconceptions about the relative likelihood of different values of the fraction of the population that prefers apple pie *before you see the results of the poll.* In contrast $\tilde{P}(F = t \mid X = 0.574)$, your judgement after you have seen the poll, is called the *posterior* probability. We will first consider the simplest approach to the prior, which is in fact often used, and then we will return to the question of how reasonable that is. The simplest solution is to assume that F is uniformly distributed, and thus $\tilde{P}(F = t)$ is a constant. In that case $\tilde{P}(F = t \,|\, X = 0.574) = \alpha \cdot B_{1000,t}(574)$ where α is a normalizing constant. This is not actually equal to the binomial distribution, which would be $B_{1000,0.574}(1000t)$, but like the binomial distribution it is accurately approximated by a Gaussian distribution with mean $\mu = 0.574$ and standard deviation $\sigma = \sqrt{0.574 \cdot (1 - 0.574)/1000} = 0.0156$. So as in our discussion above, for any q, the probability that f is between $\bar{f} - q\sigma$ and $\bar{f} + q\sigma$ is given by $2E(q) - 1$.

The advantage of the Bayesian approach is that it answers the question that we want answered: namely, what, probably, is the fraction of the population that prefers apple pie. (As we will see in section 11.4, the sample space approach refuses to answer this question.)

The weak point of the Bayesian approach is the arbitrary choice of prior. Why should we assume that F is uniformly distributed? One answer that is often given is that, once you have enough evidence, the priors don't matter. For certain kinds of priors, that is demonstrably true. For example, suppose that rather than apple pie, this poll is measuring approval ratings for the president. You might think that positing a uniform distribution on approval ratings is ignoring history; we know that approval ratings for the President are generally somewhere between 35% and 65% and almost never lower than 20% or higher than 80%. Perhaps we should use a prior that reflects that knowledge; for example, set $\tilde{P}(F = t)$ to be 1.5 for t between 0.2 and 0.8 and 0.25 for $t < 0.2$ and for $t > 0.8$. Don't even bother. When you have done all the computation, you will find that the change in the confidence interval is infinitesimal, because the posterior probability is tiny that the approval rating is outside the range $[0.2, 0.8]$. (On the other hand, if your poll does return a result of 20%, then this choice of priors will make a difference.)

But if you use a radically different model for the prior, then the choice of prior may make a difference. Suppose we choose the following probabilistic model as a prior: Define a Boolean random variable X_i expressing the pie preferences of person i; and assume that each of the X_i follows a Bernoulli distribution with its own parameter parameter p_i; the $X_i's$ are all independent; and the p_i are themselves uniformly distributed over $[0, 1]$. In this model the prior on F is a Gaussian, with norm 0.5 and with standard deviation $3.5 \cdot 10^{-5}$. You will need a vast poll to get a posterior probability that is not very close to 0.5. To put it more simply, in this model when we poll our 1000 subjects,

we get information about their personal values of p_i, but we get no information about anyone else's value of p_i, because our model says that these are all independent. You need to poll essentially everyone to get an accurate view of F.

Now, you may say that on that model, the history of opinion polls in this country is inexpressibly unlikely, which is true; and based on that fact, a sensible statistician will not choose that prior. However, from a logical standpoint this is not altogether satisfying. After all, all the other polls are also just posterior information; according to a pure Bayesian theory the proper way to consider them is to combine them with the priors that existed before ever seeing *any* polls. Simply *rejecting* a probabilistic model that makes the posterior data unlikely is essentially the hypothesis testing approach (see section 11.5) which is generally frowned on in Bayesian theories.

Moreover, in some cases you actually *do* want to use a prior that is something like this second example. For instance, consider again the problem of determining whether or not your municipality has unusually high rates of cancer. In that case, a reasonable prior might be that, in each municipality, there is some underlying probability of getting cancer, and that all these probabilities are uniformly distributed and independent from one municipality to the next. In that case, the paradox that somehow taking samples in other municipalities was affecting our judgement of this one, goes away. In this model, taking samples in other municipalities has no effect on the inference from the conclusions from the sample here.

11.4 Confidence intervals in the frequentist viewpoint: (Optional)

The interpretation of confidence intervals in the frequentist (sample space) view of probability is much more roundabout. In this viewpoint, the statement, "Based on this poll, the probability is .95 that between 54% and 60% of people prefers apple pie" is entirely meaningless, since it does not refer to any sample space. Instead, the meaning of confidence intervals is a statement about the procedure used to compute them:

Definition 11.1. *The confidence interval at level p for a sample of size n is given by a pair of monotonically non-decreasing functions $L_n(\bar{f})$ and $U_n(\bar{f})$ with the following property. Consider any property Φ whose true frequency in the space Ω is f. Let X be the random variable whose value is the number of elements with property Φ in a random sample of size n from Ω.*
Then $P(L_n(X) \leq f \leq U_n(X)) \geq p$.

That is, if you take a random sample of size n, find the fraction $\bar{f}$ of elements in the sample that are Φ and compute the values $L_n(\bar{f})$ and $U_n(\bar{f})$, then, with probability at least p, $L_n(\bar{f})$ will be less than the true frequency f and $U_n(\bar{f})$ will be greater than f.

The value of any particular confidence interval is just the application of this procedure to $\bar{f}$; e.g. when $\bar{f} = 0.574$, then $L_{1000}(\bar{f}) = 0.54$ and $U_{1000}(\bar{f}) = 0.60$.

Here the sample space Ω is the set of random samples of size n. Note that this does not make any claim whatsoever about this particular poll, or even about polls where $\bar{f} = 0.574$. It could be that all the poll questions you ever ask are actually lopsided by at least 80%-20% in the population, so that the only times you get $\bar{f} = 0.574$ are when you have, by incredibly bad luck, chosen a wildly unrepresentative sample. In that case, whenever you compute the confidence interval for $\bar{f} = 0.574$, it *never* includes the true value of f, which is either less than 0.2 or greater than 0.8. That would not at all affect the correctness of the claim being made about the confidence interval. This claim does not say that the confidence interval for $\bar{f} = 0.574$ usually, or ever, contains the true value. What it says is that, whatever poll is being carried out, for *most* random samples, this *procedure*

will give me valid bounds on the true fraction. If $f = 0.2$ then you will only very rarely get the value $\bar{f} = 0.574$.

The condition that $L(\bar{f})$ and $U(\bar{f})$ are monotonically non-decreasing is needed for the following reason. Suppose that you have come up with procedures L and U that satisfy definition 11.1. Now, some trouble-maker defines procedure L' and U' as follows:

If $\bar{f} \neq 0.574$ then $L'(\bar{f}) = L(\bar{f})$ and $U'(\bar{f}) = U(\bar{f})$.
If $\bar{f} = 0.574$ then $L'(\bar{f}) = 0.1$ and $U'(\bar{f}) = 0.2$.

Then L' and U' satisfy the condition $P(L'(X) \leq f \leq U'(X)) \geq p'$, where p' is very slightly less than p; because the odds of getting a sample fraction of *exactly* 0.574 is small even for the case $f = 0.574$. The condition that L and U are monotonically increasing excludes this kind of shenanigans.

We can go about constructing a confidence interval procedure as follows. Suppose we can find monotonically increasing functions $Q(f)$, $R(f)$ such that $P(Q(f) \leq X \leq R(f)) \geq p$ for every value of f. This is not quite what we are looking for, because the roles of f and X are reversed. Now let $U(X) = Q^{-1}(X)$ and $L(X) = R^{-1}(X)$. Since Q is monotonically increasing, $f \leq U(X)$ iff $Q(f) \leq Q(Q^{-1}(X)) = X$ and likewise $f \geq L(X)$ iff $R(f) \geq X$. Therefore

$$P(L(X) \leq f \leq U(X)) = P(R^{-1}(X) \leq f \leq Q^{-1}(X)) = P(Q(f) \leq X \leq R(f)) \geq p$$

which is what we wanted.

How can we find these functions Q and R? There is a range of acceptable possibilities, but the simplest thing is to choose $Q(t)$ such that with probability $(1-p)/2$, X is in the interval $[0, Q(f)]$ and with probability $(1-p)/2$, X is in the interval $[R(f), 1]$. Thus, with probability p, X is in neither of those intervals, and thus in the interval $[Q(f), R(f)]$. Now, nX is distributed according to the binomial distribution $B_{n,f}$. Let $C_{n,f}$ be the cumulative distribution corresponding to the binomial distribution. Then we have

$(1-p)/2 = P(0 \leq X \leq Q(f)) = C_{n,f}(n \cdot Q(f))$, so
$Q(f) = (1/n) \cdot C^{-1}_{n,f}((1-p)/2)$; and

$(1-p)/2 = P(R(f) \leq X \leq 1) = 1 - P(0 \leq X \leq R(f)) = 1 - C_{n,f}(n \cdot R(f))$ so
$R(f) = (1/n) \cdot C^{-1}_{n,f}(1 - ((1-p)/2)) = (1/n) \cdot C^{-1}_{n,f}((1+p)/2)$.

If n is large, f is not close to either 0 or 1, and p is not very close to 1, then we can make this much simpler using the Gaussian distribution. Specifically, let $\sigma = \sqrt{f(1-f)/n}$, which is the standard deviation of $\bar{f}$. Let $N_{f,\sigma}(t)$ be the Gaussian with mean f and standard deviation σ and let $E_{f,\sigma}(x)$ be the corresponding cumulative distribution. By the central limit theorem, the cumulative distribution of the Gaussian approximates the cumulative distribution of the binomial so for any k, as long as k is substantially less than $\min(f/\sigma, (1-f)/\sigma)$ we have,

$$p = P(f - k\sigma \leq X \leq f + k\sigma) \approx E_{f,\sigma}(f + k\sigma) - E_{f,\sigma}(f - k\sigma) = E_{0,1}(k) - E_{0,1}(-k) = 2E_{0,1}(k) - 1$$

so $k = E^{-1}_{0,1}(1+p)/2$. Using that value of f, we have $Q(f) = f - k\sigma$ and $R = f + k\sigma$. Finally, if n is large, so that $k\sigma \ll f$, then Q and R are very nearly inverses of one another, and we can approximate σ as $\sigma' = \sqrt{\bar{f}(1-\bar{f})/n}$ so $L(X) = R^{-1}(X) \approx Q(X)) = f - k\sigma'$ and $U(X) = f + k\sigma'$. The method for computing the confidence interval is exactly the same as in the Bayesian approach,[5] though the interpretation is very different.

[5]The Bayesian and the frequentist confident intervals are very nearly the same for large values of n and for $\bar{f}$ not close to 0 or 1; for small values of n or extreme probabilities, they can be quite different.

The advantage of the frequentist approach is that we no longer have to make any assumptions about the prior distribution of f. The answer to the frequentist question is valid whatever the prior distribution; it is valid even if, as many frequentists would claim, the idea of the prior distribution of f is meaningless. The disadvantage is that it no longer answers the question that we are interested in, "What is the actual fraction of people who prefers apple pie?"; it makes a claim about a certain statistical procedure. It is a consequence that if we follow the procedure and treat the confidence interval *as if it were* an actual statement about f, then most of the time we will be OK; but that seems like a very indirect, not to say mealy-mouthed, approach.

More importantly, for many purposes, such as computing an expected value or to calculate another probability, it is convenient to have a probability distribution over f. Now, it may be possible to rephrase these purposes as well in the probability distribution over the sample rather than over f itself, but this is always indirection, and generally difficult and problematic.

11.5 Hypothesis testing and statistical significance

A *hypothesis testing method* is a method that uses statistical characteristics of a body of data to accept or reject a particular hypothesis about the processes that generated that data.

In this section we will discuss the traditional statistical approach to hypothesis testing, which is commonly used in statistical data analysis. Like the frequentist definition of confidence intervals, this approaches the issue from a rather backward point of view. In this approach the objective of a successful (e.g. publishable) statistical analysis is formulated as *rejecting* a hypothesis, known as the *null hypothesis*, about the process that generated the data. Thus, the null hypothesis is the hypothesis that you are rooting against, so to speak. To decide whether or not to reject the null hypothesis, the statistician uses a *statistical test*, which is a Boolean function computed from the data. The hypothesis can be rejected if the outcome of the test would be very unlikely if the hypothesis were true.

Some examples of data sets, hypotheses, and tests.

1. The pie preferences of Americans are being tested. The data set is the results of the poll. What we want to prove is that most Americans prefer apple pie to blueberry pie. The null hypothesis is that the data set is the outcome of a uniform distribution over all samples of 1000 Americans; and that the fraction of Americans who prefer apple pie is at most 0.5. The statistical test is the proposition, "$0.53 \leq \text{Freq}_D(\text{Apple})$", at least 53% of the people sampled prefer apple pie.

2. A drug is being tested for its effectiveness against a disease. 30 patients who have the disease are given the drug and 30 are given a placebo. The data set is the record of which patients had recovered by the end of the week. The hypothesis you want to prove is that the drug has some effectiveness. The null hypothesis is, therefore, that it is at best useless. Specifically, that among patients who receive the drug, recovery is a Bernoulli process with parameter a; among the patients who receive the placebo, recovery is a Bernoulli process with parameter b; and $a > b$.
$$P(Recover \mid Drug) > P(Recover \mid Placebo)$$
The test T is the Boolean function,
$$\underset{D}{\text{Freq}}(Recover \mid Drug) - \underset{D}{\text{Freq}}(Recover \mid Placebo) > 0.2$$

3. You wish to show that playing Mozart to fetuses in the womb has some effect (positive or negative) on their IQ. D is a data set that records how many hours the fetus was exposed to

and what the child's IQ was at the age of 6 months. The null hypothesis is that the two data are the outcome of independent random variables. The statistical test is that the correllation between hours of Mozart and IQ score is greater than 0.2.

A test T gives good evidence for rejecting hypothesis H if positive outcomes for T are unlikely for any process Q satisfying H.

Formally, we posit the following definition.

Definition 11.2. *Let H, the* null hypothesis*, be a set of random processes, each of which generates values in a set Ω. For each process $Q \in H$, let P_Q be the probability distribution associated with the outcome of Q. Let T, the* statistical test*, be a subset of Ω (the set of samples for which the test succeeds). Let D, the* data set*, be an element of Ω. Let $s > 0$. Then H* is rejected at significance level s using T as applied to D *if $D \in T$ and $P_Q(T) \leq s$ for all $Q \in H$.*

For instance, in example 1, Ω is the set of all samples of Americans of size 1000. For any sample $s \in \Omega$ let $A(s)$ be the fraction that prefer apple pie. The null hypothesis H is the set of all binomial distributions $B_{p,1000}$ where $p \leq 0.5$. The test $T = \{s \in \Omega \mid A(s) > 0.53\}$. The data set D is the particular sample; note that $A(D) = 0.574$ so $D \in T$. Clearly over the processes $Q \in H$, $P_Q(T)$ reaches its maximum when $p = 0.5$; and for that particular Q, $P_Q(T) = 0.0275$. Therefore, the null hypothesis can be rejected at the 2.75% level.

There is an obvious problem with definition 11.2. There is nothing in the definition that prevents you from choosing T so $P_Q(T)$ is unlikely whether Q satisfies the hypothesis or not. For instance, in the pie test, we could choose as our test $T = \{s \in \Omega \mid A(s) = 0.574\}$; again, $D \in T$. This test on exact equality has probability of no more than about 1/30 whatever the actual fraction, and therefore it can be used to reject any hypothesis at all at the 0.03 significance level.

The problem is that there are two kinds of errors that can be made in hypothesis testing. The first is to reject the null hypothesis when it is in fact true; this is known as a *type 1* error. The second is to fail to reject it when it is in fact false; this is known as a *type 2* error. In general, in choosing a test for a particular hypothesis, there is a tradeoff between the two types of errors; in order to make the probability of a type 1 error small, one must accept a large probability of a type 2 error, and vice versa. Definition 11.2 ensures that it is unlikely that you will make a type 1 error, but says nothing about type 2 errors.

There is a reason for this assymetry; guarding against type 2 errors is problematic. We need to establish that if the null hypothesis is false, then it is unlikely that the test will succeed. But one cannot speak of the probability of the event T on the assumption that the sample was *not* generated by process Q. One could require that the probability of T is small given any process Q outside H; but in general the set of processes outside H is unmanageable and useless. In example 1, for instance, the process Q that generates D with probability 1 is certainly outside of H, since it is not a Bernoulli process of any kind, and $P(T|Q) = 1$.

This problem can be solved as follows:

a. Consider only a fixed space of hypotheses Ω. For instance, assume that the data was generated by a binomial distribution $B_{n,q}$ for some value of q.

b. Let H_a, the *alternative hypothesis* $= \Omega \backslash H$. Define the *power of test T over H_a* as the maximum over all tests $Q \in H_a$ of $P(\neg T|Q)$, the probability that a type 2 failure will not occur given that the data is generated by Q.

c. Consider only tests of a particular form; generally either $f(D) \geq l$ (a *one-sided* test) or $l \leq f(D) \leq u$ (a *two-sided test*) for constants l and u. (The function $f(D)$ is called a *statistic* of the data D.)

d. Require that the test T being applied satisfy the following: Of all tests T' of the form in (c) that reject the hypothesis H at level α, T should be the test that achieves the maximum power over H_a.

Thus, the test T is very unlikely to be satisfied if the data was generated by a process Q satisfying null hypothesis, but it is not inherently unlikely, in the sense that it is likely for at least some processes satisfying the alternative hypothesis.

In the apple pie example, if H is the set of all binomial distributions $B_{n,p}$ such that $p \leq 0.5$ then H_a is the set of all $B_{n,p}$ such that $p > 0.5$. Consider again the defective test T, "Reject H on sample s if and only if $A(s) = 0.574$"; thus $D \in T$. Over Q in H, the maximum likelihood of $P(T|Q)$ is achieved when $p = 0.5$ at

$$B_{1000,0.5}(0.574) \approx N_{500,15.811}(574)/15.811 = N_{0,1}(4.6802)/15.811 = 4.42 * 10^{-7}$$

so a type 1 error is extremely unlikely. However, the maximum likelihood of $P(T|Q)$ for $Q \in H_a$ is achieved when $p = 0.574$, and is only $B_{1000,0.574}(574)/ \approx N_{0,1}(0)/15.637 = 0.0155$

By contrast, consider the test T', "Reject H on sample s if $A(s) \geq 0.574$." Over Q in H, the maximum likelihood of $P(T'|Q)$ is likewise achieved when $p = 0.5$; its value is only very slightly larger than $P(T|Q)$. However, the maximum likelihood of $P(T'|Q)$ is achieved with $p = 1$ and is equal to 1.

Note that the restriction (a) above was implicitly imposed in the Bayesian analysis of confidence intervals in section 11.3. We considered a prior probability distribution over the fraction f; we did not assign any probability to the possibility that the sample was not generated by random selection.

11.6 Statistical Inference and ESP

The conflict between the frequentist and the likelihood interpretations of probability appeared in a front-page New York Times article on January 5, 2011. The circumstances were these: Prof. Daryl Bem did a number of experiments to detect precognition. For example, in one experiment, subjects were first presented with a list of 48 words to study; second, they were given a memory test on these words; third, they were given a subset of 24 of the words and asked to categorize them. (In general, people remember a list of words better if they have gone through the work of categorizing them than if they have just tried to memorize it as a list.) In Bem's experiments he found that subjects did better on the memory test on words that they spent time categorizing *after* the test was complete. Using a standard statistical measure, he determined that the null hypothesis — that the difference was entirely due to chance — could be rejected at a high level of significance.

A number of critics (e.g. Rouder and Morey, 2011) argued that, from a Bayesian point of view, it would be necessary to consider the prior probability of the hypothesis that the subjects were benefitting from extra-sensory perception, which, they stated, was very small. On this view, though some of Bem's experiments substantially raised the posterior estimate of the reality of ESP, they did not raise it to the point where reasonable people would actually believe it. The critics did not, however, give any guidance on the difficult question of how one could reasonably estimate the prior probability that ESP was possible: 10^{-8}, 10^{-50}, $10^{-10^{50}}$?

Exercises

Exercise 11.1

Using pencil and paper but no computer, estimate confidence intervals for polls over samples of sizes $N = 400$, $N = 10,000$, $N = 1,000,000$; $\bar{f} = 0.2$ and $\bar{f} = 0.5$; and confidence levels of 0.99 and 0.999. (Consider all combinations; thus your answer should have 12 parts.)

Exercise 11.2

Using MATLAB compute confidence intervals for polls over samples of sizes $N = 750$, $N = 3,500$, $N = 1,250,000$; $\bar{f} = 0.28$ and $\bar{f} = 0.65$; and confidence levels of 0.86 and $1 - 10^{-5}$. (As in exercise 1, your answer should have 12 parts.)

Problems

Problem 11.1

As mentioned in the text, the simple formula for confidence interval given in section 11.1 breaks down if N is small, $\bar{f}$ is close to 1, or a very high degree of confidence is required.

A. Consider the problem of computing a 80% confidence interval, under the frequentist definition, for the situation in which you poll 8 people and 7 respond that they prefer apple pie. Compute a confidence interval (there is more than one possible answer). Use the exact discrete distribution; do not approximate it by a continuous one.

B. (Difficult: this can be done using MATLAB but requires some care to avoid running into overflow problems.) Compute a 99% confidence interval for the situation where you poll 1000 people and 995 prefer apple pie.

Problem 11.2

Repeat problem 11.1, but using instead the Bayesian interpretation of confidence intervals, assuming a prior which is a uniform distribution over the true fraction f. Again, part (B) is difficult.

Problem 11.3

The Bayesian treatment of hypothesis testing is conceptually simpler than the frequentist idea of statistical significance; one simply computes the posterior probability that the hypothesis is true.

Suppose that you are flipping a coin. You are considering three hypotheses:

A. The coin is weighted so that it comes up heads 1/4 of the time and tails 3/4 of the time.

B. The coin is fair.

C. The coin is weighted so that it comes up heads 3/4 of the time and tails 1/4 of the time.

Assume that the prior probability of each of these is 1/3. You now flip the coin 10 times and get 7 heads. What are the probability of the three hypotheses given the results of the coin-flips?

Problem 11.4

Starting with the same priors as in exercise 11.3, suppose you flip the coin 100 times and get 70 heads. Estimate the posterior probabilities of the three hypotheses.

Problem 11.5

Suppose that as in exercise 11.3, you are flipping a coin. Let X be the bias of the coin; e.g. if $X = 1/4$ then the coin comes up heads 1/4 of the time. Suppose that your prior on X is the uniform distribution between 0 and 1. You now flip the coin 10 times and it comes up heads 7 times; call this data D. What is the posterior probability density of X; that is, $\tilde{P}(X \mid D)$? Use MATLAB to plot this curve.

Chapter 12

Monte Carlo methods

Broadly speaking, a Monte Carlo method is one that uses random choices to solve a problem. In this chapter, we will look at a particular class of methods that work by generating a large number of values within some probability space and doing a simple calculation over them. In section 12.9, we will sketch some further kinds of probabilistic algorithms and applications.

12.1 Finding area

Suppose that you want to find the area of the region defined by the inequalities $0 \leq x \leq 10, 0 \leq y \leq 10, -0.1 \leq x \cdot \sin(\pi x) \cdot y \cdot \sin(\pi y) \leq 0.1$. It is not possible to compute this as a closed form analytic expression, and it is hard work to use deterministic methods of numerical integration.

However, there is a very simple Monte Carlo method. Let R be the region satisfying the inequalities and let Q be the square $[0, 10] \times [0, 10]$. For some large N, pick N points uniformly over Q; that is choose x and y coordinates each uniformly distributed between 0 and 10. For each such point, calculate whether the point is in Q by checking whether the inequality $-0.1 \leq x \cdot \sin(\pi x) \cdot y \cdot \sin(\pi y) \leq 0.1$ is satisfied. Let K be the number of sample points in R, and let $p = K/N$. Since $R \subset Q$, the probability that any given sample point $\mathbf{x}$ is in R is just $\text{Area}(R)/\text{Area}(Q)$. Therefore K follows the binomial distribution $B_{n,p}$ where $p = \text{Area}(R)/\text{Area}(Q) = \text{Area}(R)/100$. We can therefore estimate $\text{Area}(R) = 100p$ with a standard deviation of $50\sqrt{p(1-p)/N}$. In an experiment with $N = 10000$, there were 566 points that satisfied the constraint, so the area can be estimated at 5.66, with a 95% confidence interval $[5.22, 6.10]$.

Another example: Figure 12.1 shows the case where R is the unit circle and Q is the square $[-1, 1] \times [-1, 1]$. Of 100 points chosen at random in Q, 78 are inside the circle, so the estimated area is $\text{Area}(Q) * 78/100 = 3.12$, with the 95% confidence interval $[2.64, 3.44]$. Since the true answer is $\pi = 3.14$, we were luckier in this instance than we deserved to be. An experiment with $N = 10,000$ gives a value 3.13.

Why not pick points systematically rather than randomly? Actually, for estimating the area of a two-dimensional region Q, systematically checking grid points *is* in fact a reasonable alternative to Monte Carlo methods. Pick a value of $\epsilon > 0$; construct a grid of $\epsilon \times \epsilon$ within the square Q (note that this has $N = \text{Area}(Q)/\epsilon^2$ points); count the number K of grid points in R; and estimate $\text{Area}(R)$ by $K\epsilon^2$. It is easily shown that, for any fixed R, the maximal error in this approach is $\Theta(\epsilon) = \Theta(1/\sqrt{N})$ — thus, comparable to the error in Monte Carlo search — and the result is guaranteed, rather than merely probabilistic.

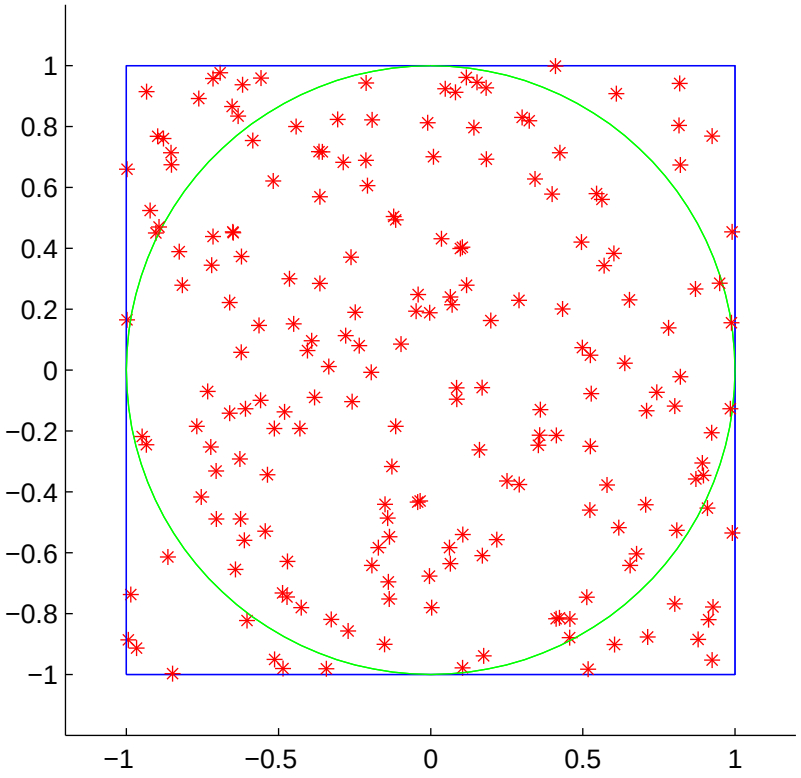


Figure 12.1: Monte Carlo estimate of the area of a circle

But there are two drawbacks. The first is that the result is asymptotic and order of magnitude. The error in the estimate is, in general proportional to the circumference of R, so unless you can bound that in some way, there is no way to know how large to choose N to get a given accuracy. If R has a sufficiently convoluted shape, it may be necessary to choose a very large value of N to get an accurate answer. Furthermore, if you don't know anything about R, then there is the fear that your systematic method of picking points may be related to the shape of R in a way that throws off the estimate.[1] For instance in the above (contrived) example, if you choose as grid the points with integer coefficients in $1 \ldots 10$, all of them satisfy the inequality, so you would estimate Area(R) at 100. With Monte Carlo search, by contrast, the accuracy of the estimate is given by the standard confidence interval, and depends on N and on Area(R), but not on any other characteristic of R.

The second drawback is that using grid points is only competitive in two dimensions. In k-dimensions the error in the grid estimate is still $O(1/\epsilon)$ but this is now $N^{-1/k}$, whereas the error in the Monte Carlo estimate is $O(N^{-1/2})$ regardless of the dimension.[2] In large number of dimension, the grid method is hopeless; for example in 100 dimensional space, a $2 \times 2 \ldots \times 2$ grid has 2^{100} points. But the Monte Carlo method doesn't care; it has exactly the same accuracy even if the dimensionality of the space is much greater than the number of sample points.

However, there is a catch; we need to be able to find an enveloping region Q satisfying the following conditions:

- We can compute Area(Q) accurately.
- We can generate points uniformly within Q;
- $R \subset Q$;
- Area(Q)/Area(R) is not very large.

In large dimensional space, this can be difficult, even if R is a quite reasonable shape. For example, suppose that R is the 100-dimensional sphere, and we try to estimate its volume using the cube $[-1, 1]^{100}$ as Q. It worked well in two dimensions, but in 100 dimensions, the ratio $\text{Area}(R)/\text{Area}(Q) = \pi^{50}/(2^{100} \cdot 50!) \approx 10^{-68}$. So we would have to generate 10^{68} points at random in the cube before finding a single one that fell in the sphere. If one wants to do Monte Carlo simulation in a large dimensional space, therefore, it is necessary to have techniques for finding regions that fit the target closely, and generating points uniformly in these.

12.2 Generating distributions

In Monte Carlo search, it is often important to generate a *non-uniform* distribution. The built-in `rand` function, however, is designed to generate a uniform distribution over [0,1]. It is therefore often necessary to turn this uniform distribution into a non-uniform distribution.

To generate a uniform distribution over the finite set $\{0 \ldots n-1\}$, use `floor(n*rand)`.

To generate a finite, non-uniform distribution with probabilities $p_1 \ldots p_k$, partition the unit interval into subintervals of length $p_1 \ldots p_k$. Let $b_0 = 0$; $b_1 = p_1$; $b_2 = p_1 + p_2$; $b_3 = p_1 + p_2 + p_3$; $\ldots b_k = 1$. If random variable U is uniformly distributed between 0 and 1, then the event $b_{i-1} \leq U \leq b_i$ has

[1] Unless R is a pathological set like the set of all points with rational coordinates — technically, if R is bounded and either topologically open or topologically closed — then it is always the case that any *sufficiently* fine uniform grid will give an accurate estimate.

[2] In *one* dimension, the grid estimate, with an error of $O(1/N)$, beats Monte Carlo.

probability p_i. Thus, to generate this distribution, you precompute the values $b_0 \ldots b_k$, you execute `rand` and you find the subinterval that contains the value returned by `rand`.

To turn a uniform distribution into a continuous, non-uniform distribution, you use the inverse of the cumulative probability. (The finite case described in the previous paragraph is actually a special case of this.) Suppose that X is a random variable with cumulative probability function $F(t)$; that is $P(X \leq t) = F(t)$. Let $u = F(t)$; then $P(X \leq F^{-1}(u)) = P(F(X) \leq u) <= u$. Thus $F(X)$ is uniformly distributed; so $X = F^{-1}(U)$ where U is uniformly distributed.

For example, suppose you want to generate points according to the density function $f(t) = e^{-t}, t \geq 0$. The cumulative probability function is $\int_0^x e^{-t}dt = 1 - e^{-x}$. If $y = 1 - e^{-x}$, then $x = -\ln(1-y)$. So you generate values of a random variable Y uniformly between 0 and 1, compute $X = -\ln(1-Y)$, and then $\tilde{P}(X = t) = e^{-t}$.

Likewise, if you want to generate points with the distribution $f(t) = 1/t^2, t \geq 1$, then the cumulative function is $1 - 1/x$. The inverse is the function $x = 1/(1-y)$. So if Y has the uniform distribution from 0 to 1, then $X = 1/(1-Y)$ has the p.d.f. $1/t^2$.

Computing the inverse of the cumulative function for the Gaussian is not so simple. Luckily, MATLAB has a built-in function `randn` which generates random variables according to the standard normal distribution $N_{0,1}$.

12.3 Counting

Essentially the same technique that we have used for estimating area can be used to estimate the size of a finite set R. To estimate R, find a set Q such that

- $R \subset Q$.
- $|Q|$ is easily computed.
- It is easy to generate random elements uniformly in Q.
- $|R|/|Q|$ is not very small.

In that case, generate a sample of N points uniformly in Q; let K be the number of points in the sample that lie in R; let $p = K/N$; and estimate $|R|$ as $p|Q|$, with a standard deviation of $\sqrt{p(1-p)/N}$ where $p = K/N$.

For instance, suppose that you want to estimate the number of integer solutions $\langle x, y, z\rangle$ to the constraints:

$0 \leq x \leq W$; $0 \leq y \leq W$; $0 \leq z \leq W$.
$x^2 + x + y^2 + y + z^2 + z + 1$ is a prime number.

for various values of W. This can be estimated as follows:

- Generate N random triples $\langle x, y, z\rangle$ of integers between 0 and W, using independent, uniform distributions for each.
- Count the number K of triples satisfying the condition that $x^2 + x + y^2 + y + z^2 + z + 1$ is a prime number. Let $p = K/N$.
- Since there are $(W+1)^3$ triples in total, estimate the total number of triples as $p \cdot (W+1)^3$, with a standard deviation of $\sqrt{p(1-p)/N}(W+1)^3$.

Since the number of prime numbers less than Q is $Q/\ln Q$, it should be possible to get an estimate accurate within a factor of $1+\delta$ by generating $O(\ln N/\delta^2)$ points.

12.4 Counting solutions to DNF (Optional)

An interesting example of a counting problem that can be solved using Monte Carlo methods is finding the number of solutions to a formula in disjunctive normal form (DNF).[3] A propositional formula ϕ is in DNF if it is expressed as the disjunction of a collection of conjunctions of literals, where a literal is either a propositional atom or its negation. For example, the following formula is in DNF:

$$(A \wedge B \wedge \neg C \wedge \neg D) \vee (\neg A \wedge \neg B) \vee (\neg B \wedge C) \tag{12.1}$$

Let $\mu_1 \ldots \mu_k$ be the conjunctions in ϕ. Let m be the total number of propositional atoms in ϕ. For example, in formula 12.1, $m = 4$ (A, B, C, and D), $k = 3$ and $\mu_1 = A \wedge B \wedge \neg C \wedge \neg D$, $\mu_2 = \neg A \wedge \neg B$, $\mu_3 = \neg B \wedge C$.

A valuation — that is, an assignment of T or F to each atoms — satisfies a formula ϕ in DNF if it satisfies *all* of the literals in *at least one* of the μ_i. For example, the valuations that satisfy the above formula are:

$\langle A = T, B = T, C = F, D = F \rangle$ — satisfies μ_1.
$\langle A = T, B = F, C = T, D = T \rangle$ — satisfies μ_3.
$\langle A = T, B = F, C = T, D = F \rangle$ — satisfies μ_3.
$\langle A = F, B = F, C = T, D = T \rangle$ — satisfies both μ_2 and μ_3.
$\langle A = F, B = F, C = T, D = F \rangle$ — satisfies both μ_2 and μ_3.
$\langle A = F, B = F, C = F, D = T \rangle$ — satisfies μ_2.
$\langle A = F, B = F, C = F, D = F \rangle$ — satisfies μ_2.

So there are seven valuations that satisfy formula 12.1.

The abstract problem of counting the solutions to a DNF formula has a number of important practical applications. For example, if you have a network where individual edges can fail with a specified probability, and you want to know the probability that two nodes will be able to communicate, then that problem can be expressed in terms of the number of solutions to a particular DNF formula. However the problem is what is called "#P-complete" (read "sharp P complete"). The class of #P-complete problems bears the same relation to the space of counting problems as the relation of the class of NP-complete problems to the space of decision problems; as far as anyone knows, no polynomial-time exact solution exists. However, there is an efficient Monte Carlo algorithm that gives a probabilistic, approximate solution for counting the solutions to a DNF formula.

The obvious way to construct a Monte Carlo algorithm here would be to take the target set R here is the set of all valuations satisfying the formula, and the enveloping set Q to be the set of all 2^m valuations over the m atoms. However, that does not work; there are cases — and, moreover, cases of practical importance — where $|R|$ is exponentially small as compared to $|Q|$. We have to be cleverer.

Instead, we take the enveloping set Q to be the set of all pairs $\langle s, i \rangle$ where i is an index between 1 and k, and where s is a valuation satisfying μ_i. We take the set R to be the subset of S, which is the set of all pairs $\langle s, i \rangle$ where s is any valuation satisfying ϕ and where i is the smallest index for which s satisfies μ_i.

[3] This algorithm is from (Karp, Luby, and Madras, 1989).

For example, in formula 12.1, the enveloping set Q is

$$\begin{aligned} Q = \{\ & \langle\langle A=T, B=T, C=F, D=F\rangle, 1\rangle, \\ & \langle\langle A=T, B=F, C=T, D=T\rangle, 3\rangle, \\ & \langle\langle A=T, B=F, C=T, D=F\rangle, 3\rangle, \\ & \langle\langle A=F, B=F, C=T, D=T\rangle, 2\rangle, \\ & \langle\langle A=F, B=F, C=T, D=T\rangle, 3\rangle, \\ & \langle\langle A=F, B=F, C=T, D=F\rangle, 2\rangle, \\ & \langle\langle A=F, B=F, C=T, D=F\rangle, 3\rangle, \\ & \langle\langle A=F, B=F, C=F, D=T\rangle, 2\rangle \\ & \langle\langle A=F, B=F, C=F, D=F\rangle, 2\rangle \\ \} & \end{aligned}$$

The target set R is

$$\begin{aligned} R = \{\ & \langle\langle A=T, B=T, C=F, D=F\rangle, 1\rangle, \\ & \langle\langle A=T, B=F, C=T, D=T\rangle, 3\rangle, \\ & \langle\langle A=T, B=F, C=T, D=F\rangle, 3\rangle, \\ & \langle\langle A=F, B=F, C=T, D=T\rangle, 2\rangle, \\ & \langle\langle A=F, B=F, C=T, D=F\rangle, 2\rangle, \\ & \langle\langle A=F, B=F, C=F, D=T\rangle, 2\rangle \\ & \langle\langle A=F, B=F, C=F, D=F\rangle, 2\rangle \\ & \} \end{aligned}$$

That is, in this case R contains all the pairs in Q except the two pairs $\langle\langle A=F, B=F, C=T, D=T\rangle, 3\rangle$, and $\langle\langle A=F, B=F, C=T, D=F\rangle, 3\rangle$, because those valuation satisfy μ_2 as well.

Now note that

- Any valuation that satisfies ϕ appears exactly once in R; namely associated with the first μ_i that it satisfies. Therefore, $|R|$ is the number of valuations satisfying ϕ.
- Any valuation appears at most k times in Q. Therefore $|R|/|Q| \geq 1/k$.
- If we have chosen a pair $\langle s, i\rangle$ from Q, we can check whether it is in R by looping through the conjunctions $\mu_1 \ldots \mu_{i-1}$ and seeing if s satisfies any of these. This can be done in time $O(|\phi|)$.

What remains is to come up with a method for picking elements of Q uniformly. That is done as follows: We will first choose i, then choose s. We will how these are done in the opposite order:

Suppose we have chosen a particular conjunction μ_i. This has the form $\mu_i = \lambda_1 \wedge \ldots \wedge \lambda_{r_i}$ for some value of r_i. So the atoms in $\lambda_1 \ldots \lambda_{r_i}$ must have the values indicated by the λ's, and the other atoms can have any combination of values. Therefore there are 2^{m-r_i} different valuations satisfying μ_i; and we can pick one of these at random just by giving all the atoms in $\lambda_1 \ldots \lambda_r$ the right value, and assigning the other atoms values T or F with probability 1/2.

For example, in formula 12.1, if we choose $i = 3$ then $\mu_3 = \neg B \wedge C$, so $r = 2$. So there are $2^{4-2} = 4$ valuations satisfying μ_3. We can select a random valuation by choosing $B = F$ and $C = T$; picking $A = T$ or $A = F$ randomly with probability 1/2; and picking $D = T$ or $D = F$ randomly with probability 1/2.

Thus, the number of pairs in Q with index i is 2^{m-r_i}, so the total number of pairs in Q is $|Q| = \sum_i^k 2^{m-r_i}$. Therefore, if we want to pick pairs in Q uniformly, we should pick index i with probability $p_i = 2^{m-r_i}/|Q|$.

function CountDNF(**in** ϕ: A formula in DNF; n: number of Monte Carlo iterations)
return An estimate of the number of valuations satisfying ϕ

```
/* Preprocessing */
{ m ← the number of propositional atoms in φ;
  μ_1 ... μ_k ← the conjuncts in φ;
  for (i = 1 ... k) r_i ← the number of literals in μ_i;
  for (i = 1 ... k) C_i ← 2^(m−r_i);
  |Q| = Σ_{i=1}^{k} C_i;
  for (i = 1 ... k) p_i = C_i/|Q|;

/* Monte Carlo loop */
  Count ← 0
  for (j ← 1 ... n)
      pick i at random, following distribution p_i;
      construct a random valuation s satisfying μ_i
          by setting all the atoms in μ_i as specified there
          and setting all the other atoms to be T/F with probability 1/2;
      SinR ← true;
      for (w ← 1 ... i − 1)
          if s satisfies μ_w then { SinR ← false; exitloop } endif;
      endfor
      if SinR then Count ← Count + 1 endif
  endfor

  return Count * |Q|/N;
}
```

Table 12.1: Monte Carlo algorithm to count the number of solutions to a formula in DNF

For example, in formula 12.1, we have $m = 4, r_1 = 4, r_2 = 2, r_3 = 2$ so $|Q| = 2^0 + 2^2 + 2^2 = 9$ and $p_1 = 2^0/|Q| = 1/9$, $p_2 = 4/9$; $p_3 = 4/9$. Thus, there is a 1/9 probability that we will choose $i = 1$ and therefore a 1/9 probability that we will choose the single valuation satisfying with μ_1; there is a 4/9 probability that we will choose $i = 2$, and, having done so, a 1/4 probability of choosing each of the 4 valuations satisfying μ_2 for a total probability of 1/9 for each of these; and likewise for $i = 3$. Therefore each element of Q has a 1/9 probability of being selected, as promised.

Putting all this together, we get algorithm CountDNF shown in table 12.1

12.5 Sums, expected values, integrals

If Q is a set and f is a numeric function over Q, you can estimate $\sum_{x \in Q}$ as $(|Q|/|S|) \cdot \sum_{x \in S} f(x)$ where S is a random sample of Q.

If Q is a numerical random variable, then you can estimate $\text{Exp}(Q)$ by taking a sample of Q of size n and computing the average over those sample. You can estimate $\text{Std}(Q)$ by computing the standard deviation of the sample.

If f is an integrable function over $\mathbb{R}^k$ and Q is a region in $\mathbb{R}^k$ then you can estimate $\int_Q f(t)dt$ as $\sum_{x \in S} f(x) \cdot \text{Area}(Q)/|S|$, where S is a random sample of points in Q. The method of computing the

area of region R in section 12.1 is actually a special case of this, where Q is the enveloping region, and $f(x)$ is the characteristic function of R — that is, $f(x) = 1$ for $x \in R$ and 0 for $x \notin R$.

The accuracy of all these is generally proportional to $1/\sqrt{n}$ where n is the sample size. The constant of proportionality depends on the characteristics of the example.

A couple of caveats should be mentioned.

The technique does not work in the case where there is a very small region where f is immensely larger than everywhere else. Specifically, for computing a sum over a finite set Q, suppose that there is a subset Z of Q such that:

- $|Z|/|Q| < \epsilon$.
- The average value of $f(x)$ over Z is at least on the order of $1/\epsilon$ times the average value of $f(x)$ over $Q \setminus Z$. Therefore the sum of f over Z is at least comparable to the sum of f over $Q \setminus Z$.

Then if the size of the sample is $o(1/\epsilon)$, the sample will probably not contain any elements of Z. The average size of elements in the sample will be about the average size on $Q \setminus Z$

For all of these, if there is a subset B of relative size ϵ over which f is very large ($\Omega(1/\epsilon)$) then n has to be at least several times $1/\epsilon$, in order to be confident that the sample contains a representative number of elements from B. If f follows a power-law distribution, where the top few elements have most of the total f, then a random sample is likely to be very inaccurate. You can be sure that guaranteed that this condition does not arise if either

a. The ratio between $\max_{x \in Q} f(x)$ and $\min_{x \in Q} f(x)$ is not very large; or

b. The space of y such that $f(y)$ is close to $\max_{x \in Q} f(x)$ is not very small.

These are made precise in the literature on Monte Carlo methods.

Moreover, to ensure that the estimate of $\mathrm{Exp}(Q)$ approaches its true value with probability 1 as the sample size goes to infinity, $\mathrm{Var}(X)$ must be finite. To assure that this holds for $\int_Q f(t)dt$, the integral $\int_Q f^2(t)dt$ must be finite.

Finally, if f is a well-behaved function, then deterministic methods of numerical integration give answers that are much more accurate than Monte Carlo methods, for a given amount of computation. Monte Carlo methods for integration win out for functions that, though integrable, are not well-behaved.

12.6 Probabilistic problems

Not surprisingly, Monte Carlo methods can be very effective at solving complex probabilistic problems. For example, suppose that you are interested in a particular form of solitaire, and you want to know how frequently you end up winning, with some specified strategy. It would almost certainly be hopeless to try to do an exact combinatorial analysis. However, Monte Carlo testing is comparatively easy: Program up the game and the strategy; generate 10,000 shuffles of the deck at random; and test.

One of the nice features of this example is that you can be sure at the start that the probability is not either very close to 0 or very close to 1, because forms of solitaire in which the player nearly always wins or nearly always loses usually do not survive.

Monte Carlo search can be applied in the same way to multi-player card games. Suppose that you are playing 5-card draw in poker against three other players. You want to know what the probability is that you are holding the winning hand. The Monte Carlo solution is simple: Carry out N random deals of the remaining cards to the other players, and check the fraction in which you have the winning hand.

Moreover, the strategy is easy to adapt it to a new game. Suppose one of your fellow players calls for some ridiculous variant: Two cards are visible, red jacks are wild, twos can count as aces, and if the total points in your hand is exactly equal to 43, then that beats anything. You could be working for a week trying to come up with an exact analysis of the combinations. But the Monte Carlo approach can be up and running in minutes, as long as:

- You can easily generate random hands that satisfy the known information. In poker, ignoring the information from the bets, this is just a matter of randomly dealing the invisible cards.
- You can easily calculate whether one hand beats another.

Likewise, bridge-playing programs work by doing a Monte Carlo search over distributions of the unseen cards and finding the move that most often leads to a successful outcome (Ginsberg, 1999).

The same applies outside the game context, in all kinds of complex or dynamic probabilistic situations. In financial applications, for example, the value of a portfolio of investments may be affected by a series of external events, with complex dependencies. In such cases, it may be much more effective to run a Monte Carlo simulation, generating a large random collection of scenarios, than to attempt an analytic analysis.

Problems involving continuous distributions can be addressed in this way as well. Suppose that X is a random variable with distribution $N_{5,0.2}$, and Y is a random variable uniformly distributed over $[3, 7]$. What is $P(X \cdot Y > 20)$? If you have a collection of n points in the plane where the x-coordinate is drawn from X and the y-coordinate is drawn from Y, and you draw an edge between every pair of points that are less than d apart, what is the probability that the resultant graph is connected? For the first problem, with enough hard work you can probably formulate and evaluate a definite integral. For the second, the exact analysis is certainly very difficult, and quite possibly hopeless. In this case, or similar cases, if a high degree of accuracy is not required, then a Monte Carlo evaluation can be quickly programmed up and executed, and with very high probability it will give a reasonably accurate answer.

12.7 Resampling

A method of statistical analysis that has recently become popular is called *resampling* or *non-parametric statistics*. In resampling, statistical analysis is carried out by doing Monte Carlo tests over subsamples of the data or other collections directly derived from the data. Resampling has two advantages over traditional statistics. First, many traditional statistical methods require strong assumptions about the processes that generated the data (e.g. that the data was generated by a normal distribution); resampling methods make no such assumptions. Second, traditional statistical analysis often requires complex mathematical analysis, and the use of obscure special functions; resampling techniques are much simpler to learn, to program, and to apply.

For example,[4] suppose that you want to determine whether a drug is more effective than a placebo. You have measured the improvement on a scale from 0 to 100 for a number of trials of both; the results are:

[4] These examples are taken from (Shasha and Wilson, 2008).

Placebo: 54 51 58 44 55 52 42 47 58 46
Drug: 54 73 53 70 73 68 52 66 65

Eyeballing it, it certainly *looks* like the drug is effective. The placebo has numbers in the 40's and 50's; the drug has numbers in the 50's, 60's and 70's. The average for the drug is 63.67 and the average for the placebo is 50.70; the difference between the averages is thus 9.97. But is this actually a significant difference? We carry out the following experiment: We take the same data points, but we shuffle the labels "Placebo" and "Drug" randomly. For instance, here is one reshuffling:

54-P 51-D 58-D 44-P 55-D 52-P 42-P 47-P 58-P 46-D
54-P 73-D 53-D 70-D 73-D 68-P 52-P 66-P 65-D

Here, the average for label "D" is 60.44 and the average for label "P" is 53.7. Testing 10,000 different relabellings, then the difference between the average for label "D" and the average for label "P" in only 8 cases. That establishes with a high degree of confidence that the drug *is* indeed effective; if the choice between drug and placebo were actually independent of the improvement measure, then the chances with this data of getting a difference as large as 9.7 seems to be less than 0.001.

The structure here, it may be noted, is rather different than in our previous examples. Roughly speaking the target set R here is the set of labellings where the different in mean is at least 9.7 and the enveloping set Q is the set of all relabellings. But here we are *not* interested in an accurate measure of R; all we want to do is to establish that it is much smaller than Q.

We next want to get a confidence interval for the *magnitude* of the difference between the drug and the placebo (the previous experiment only established the *existence* of a difference.) The method used is called "bootstrapping". We assume that our data for the drug is a random sample of size 9 out of a large space of results for the drug. What is that large space? The simplest assumption is that it is *exactly the same as the data we have*, repeated a zillion times. A sample from this space is just a sample of size 9 from the drug data *with replacement;* that is, some values may appear multiple times and some values may appear zero times. So to find a 90% confidence interval, what we do is to take 10,000 pairs of $\langle$ a sample from the drug data and a sample from the placebo data $\rangle$; compute the difference of the means for each such pair; sort all these differences; and find the 5% and the 95% percentile levels on all these differences. For this particular data, we find a confidence interal of [7.5, 18.1].

Be careful not to get confused about the two different kinds of samples here. At the object level, there are the samples of drug data (size 9) and of placebo data (size 10). At the meta-level, there are the bootstrap samples — 10,000 of these, each of which is a pair of a hypothetical sample of drug data and a sample of placebo data. The samples discussed in chapter 11 correspond to the object-level samples here. In particular, the width of the confidence interval is determined by the size of the object level samples (9 and 10) and *not* by the size of the bootstrap sample. As you make the bootstrap sample larger, the confidence interval does not shrink, you just get a better estimate.

12.8 Pseudo-random numbers

A limitation on Monte Carlo methods is that a function like MATLAB's `rand` is not a truly random process; it is a pseudo-random number generator. These generally work by taking an arbitrary starting value `x` called the *seed*, and then returning `f(x)`, `f(f(x))`, `f(f(f(x)))` ... for some carefully selected generator function `f`. Therefore, after a certain point they cycle.

The use of pseudo-random numbers in Monte Carlo search can give rise to two kinds of problems:

A. There could be some relation between the generator function `f` and the phenomenon being studied, so that the phenomenon is not independent of the random number stream.

B. If the Monte Carlo search involves a very large sample, then the cyclic period of the random number generator can be reached. This problem places a limit on the precision of results attainable through Monte Carlo search, particularly because one needs to generate a sample whose size is proportional to the inverse square of the desired accuracy.

Both of these problems can arise in practice. See (Fishman 1996, chapter 7) for an extensive discussion.

Random sequences that come from hardware random number generators, which are based on physical random processes, do not suffer from these problems.

12.9 Other probabilistic algorithms

Monte Carlo methods were pioneered for solving physics problems too difficult to be solved analytically; and much of the subsequent development has likewise been aimed at these kind of problems. (Indeed the method was first extensively used in the Manhattan project, which built the first atomic bomb.)

Many successful search techniques, such as simulated annealing, WALKSAT, genetic algorithms, and random restart use an element of random choice to escape local minima or wander around local plateaus. See (Russell and Norvig 2009) for an introduction to this active area of research.

In algorithmic analysis and theory of computation, if D is a decision problem (i.e. a problem with a yes/no answer) then a probabilistic algorithm A for D is one that makes a number of random choices, and has the properties that:

- If the answer to D is "true" then A always returns "true".
- If the answer to D is "false" then there is at least a 50% chance that A will return "false", where the probability is over the sample space of random choices made.

Therefore, if you run A k times and it returns "false" on any of those runs, the answer must be "false". Moreover, if the answer is false, then the probability is at most 2^{-k} that A will return "true" every time. Therefore, if you have run A k times and gotten "true" every time, then you can be reasonably (though never entirely) sure that the answer is indeed "true".

12.10 MATLAB

The function `rand` with no arguments generates a random number uniformly between 0 and 1. The function call `rand(n)` generates a $n \times n$ matrix of random numbers, independently chosen uniformly between 0 and 1. The function call `rand(m,n)` generates an $m \times n$ matrix of random numbers.

The function `randn` generates a random number distributed according to the standard Gaussian distribution $N_{0,1}$. The function calls `randn(n)` and `randn(m,n)` generate matrices.

```
>> rand
ans =
```

```
    0.3816

>> rand
ans =
    0.7655

>> rand(1,7)
ans =
    0.7952    0.1869    0.4898    0.4456    0.6463    0.7094    0.7547

>> rand(4)
ans =
    0.2760    0.1190    0.5853    0.5060
    0.6797    0.4984    0.2238    0.6991
    0.6551    0.9597    0.7513    0.8909
    0.1626    0.3404    0.2551    0.9593

% The function randn generates random numbers according to the normal
% distribution with mean 0 and standard deviation 1.

>> randn
ans =
    0.0859

>> randn
ans =
   -1.4916

>> randn(1,7)
ans =
   -0.7423   -1.0616    2.3505   -0.6156    0.7481   -0.1924    0.8886
```

It is often useful to be able to get the same sequence of random numbers; for example, in debugging. To do this, carry out the following operations:

- Create a stream `s` of random numbers, as shown below.
- Make it the default stream. Thus, this is the stream that functions like `rand` will consult.
- When you want to restart the same sequence over again, call `reset(s)`.
- If you want to go back to an intermediate state of a random stream, save the state by saving `s.State` in a variable and restore it by assigning to `s.State` from the variable where you have saved it.

```
>> s=RandStream('mt19937ar')            % Create a random stream
s =
mt19937ar random stream
             Seed: 0
         RandnAlg: Ziggurat

>> RandStream.setDefaultStream(s)       % Make it the default stream
```

```
>> rand(1,7)                  % Generate some random numbers
ans =
    0.8147    0.9058    0.1270    0.9134    0.6324    0.0975    0.2785

>> rand(1,5)                  % Generate more random numbers
ans =
    0.5469    0.9575    0.9649    0.1576    0.9706

>> state2=s.State;            % Save the current state in state2

>> rand(1,6)                  % Generate more random numbers
ans =
    0.9572    0.4854    0.8003    0.1419    0.4218    0.9157

>> reset(s)                   % Go back to the beginning

>> rand(1,7)
ans =
    0.8147    0.9058    0.1270    0.9134    0.6324    0.0975    0.2785

>> s.State=state2;            % Jump ahead to state2.

>> rand(1,6)
ans =
    0.9572    0.4854    0.8003    0.1419    0.4218    0.9157
```

MATLAB Exercises

Exercise 12.1

Use a Monte Carlo method to estimate the size of the ellipse $x^2 + xy + y^2 \leq 1$. Note: this lies inside the rectangle $[-2, 2] \times [-2, 2]$. Give the 95% confidence interval for your answer.

Exercise 12.2

An integer is *square-free* if its prime factorization consists of distinct primes. For example, 35=5*7 is square-free; 12=2*2*3 is not square free. Use a Monte Carlo method to estimate what fraction of integers less than 1,000,000 are square-free. The MATLAB function `factor(N)` computes the prime factorization of integer N. Give the 95% confidence interval for your answer.

Exercise 12.3

Use a Monte Carlo method to estimate the probability that a random string of 200 integers between 0 and 9 contains a consecutive subsequence of 5 increasing values; e.g. 2,3,6,8,9. Give the 95% confidence interval for your answer.

Problems

Problem 12.1

(This refers to assignment 12.2). In assignment 12.2 below, we write the main body of the routine as

(Version 1)

```
for I=1:N1
  use RandomWord Q times to generate a set S of word ranks;
  for I=1:N2
     count = count + (RandomWord() in S);
  end
end
```

Two possible alternatives would use only one level of looping, though the same total number of iterations of the inner loop:

(Version 2)

```
use RandomWord Q times to generate a set S of word ranks;
for I=1:(N1*N2)
     count = count + (RandomWord() in S);
  end
end
```

(Version 3)

```
for I=1:(N1*N2)
     use RandomWord Q times to generate a set S of word ranks;
     count = count + (RandomWord() in S);
  end
end
```

A. Discuss the pros and cons of these three versions in terms of running time and accuracy.

B. Suppose that it is necessary to assert a confidence interval on the answer p that corresponds to a sample of size `N1` $*$ `N2`. Which of these should be used? Why?

Programming assignments

Assignment 12.1

Implement the algorithm described in section 12.4. That is, write a function `CountDNF(F)`. The input parameter `F` is an $m \times n$ array, where n is the number of propositional atoms and m is the number of conjunctions. `F[i,j]=1` if `j` is a conjunct in μ_i; `F[i,j]=`-1 if $\neg$`j` is a conjunct in μ_i; and `F[i,j]=0` if `j` does not appear in μ_i. Thus, the input matrix for equation 12.1 would be

$$\begin{bmatrix} 1 & 1 & -1 & -1 \\ -1 & -1 & 0 & 0 \\ 0 & -1 & 1 & 0 \end{bmatrix}$$

The function should return an estimate of the number of valuations satisfying the formula.

Assignment 12.2

The values for p in table 9.4 were generated using a Monte Carlo simulation. Write a function `AlreadySeen(Q)` that carries out a comparable calculation; namely, given a subfunction `RandomWord()` that generates random word ranks, and the number of words already seen `Q`, compute the probability that the new word you see is one you have already seen.

Step 1: Write the function `RandomWord()` to follow the distribution used in table 9.4; for $I = 1 \ldots 100,000$, the probability that `RandomWord` returns I is $1/(I * H(100,000))$. Here the normalizing factor $H(N)$ is the harmonic function $\sum_{I=1}^{N} 1/I$.

Hint: Use the technique described in section 12.2 for generating finite distributions. Note that $P(\texttt{RandomWord} \leq K) = H(K)/H(100,000)$. A brute force approach is simply to compute $P(\texttt{RandomWord} \leq K)$ for $K = 1 \ldots 100,000$, save the results in an array, and then use binary search on the array to find the proper subinterval. A cleverer way that is both more time and space efficient is to precompute these values up to $K = 1000$ and then to use the fact that, for $K > 1000$, to sufficient accuracy $H(K) \approx \ln(K) + \gamma$, where γ is Euler's constant 0.5772 (see assignment 2.2). In either case, the precomputation should be done *once* and saved in a global variable; it should not be done each time `RandomWord` is called.

Step 2: Implement the following pseudo-code

```
function P = AlreadySeen(Q)
  count = 0;
  for I=1:N1
    use RandomWord Q times to generate a set S of word ranks;
    for I=1:N2
       count = count + (RandomWord() in S);
    end
  end
  P=count/(N1*N2);
end
```

Here `N1` and `N2` are reasonably large parameters that govern the Monte Carlo search.

Assignment 12.3

The "Aces Up" form of Solitaire is played with a standard deck of 52 cards and has the following rules.

```
deal four cards face up on the table;
the remaining 48 cards are the deck (face down);
repeat until (the deck is empty) {
  while (two or more visible cards have the same suit)
     discard all but the highest card of that suit;
  if (there is any empty space)
      move the top card from any other pile into that space; ***
    else deal one card from the deck face-up onto each pile;
 }
```

The player wins if at the end, only the aces remain and the other 48 cards have been discarded.

Note that at the step marked by asterisks above, the player can make a choice; hence there is some element of strategy.

Consider the following four strategies for executing the starred step.

1. Choose randomly among the remaining piles with at least 2 cards.
2. Take a card from the deepest pile.
3. Take a card from the shallowest pile with at least 2 cards.
4. If there any moves that will allow you to make a discard, then choose randomly among such moves. If not, choose randomly among the piles with at least 2 cards.

Using Monte Carlo search, for each of the strategies, compute (A) the probability of winning; (B) the expected number of cards discarded.

Assignment 12.4

Write a program uses Monte Carlo search to estimate the probability you hold a winning hand in poker, assuming that

- Every player has been dealt 5 cards.
- You can see all your own cards.
- You can see K of each of your opponents' cards.

That is, write a function `WinningPokerHand(My,Theirs)` where:

- `My` is a 2×5 array. `My[1,J]` is the number value of the Jth card. `My[2,J]` is a number from 1 to 4 indicating the suit of the Jth card (clubs, diamonds, hearts, spades).
- `Theirs` is a three-dimensional $N \times 2 \times K$ array indicating the visible cards of your opponents. N is the number of opponents. `Theirs[I,1,J]` and `Theirs[I,2,J]` are the number and suit of the Jth visible card of Ith opponent. The ace should be input as 1, though of course it can count as either 1 or 14.

For example, suppose that you hold the 3 of clubs, the 3 of spades, the queen of diamonds, the queen of spades, and the 10 of clubs. You have two opponents, and $K = 3$. The visible cards of opponent 1 are the ace of spades, the jack of spades, and the 4 of spades. The visible cards of opponent 2 are the king of diamonds, the king of spades, and the 6 of hearts. Then the input parameters are:

$$\texttt{My} = \begin{bmatrix} 3 & 3 & 12 & 12 & 10 \\ 1 & 4 & 2 & 4 & 1 \end{bmatrix} \qquad \texttt{Theirs} = \left[\begin{bmatrix} 1 & 11 & 4 \\ 4 & 4 & 4 \end{bmatrix} \begin{bmatrix} 13 & 13 & 6 \\ 2 & 4 & 3 \end{bmatrix} \right]$$

Carry out a Monte Carlo search by randomly dealing the hidden cards to the opponents from the rest of the deck, and calculating whether you have the winning hand. The function should return an estimate of the probability that you have a winning hand.

Assignment 12.5

Use Monte Carlo search to solve the following variant of the problem discussed at the end of section 12.6. Write a function **CloselyConnectedPoints(N,D)** to estimate the probability that N points chosen at random and connected with an arc of length D form a connected graph. Specifically:

A. Choose N points randomly, with the X and Y coordinates generated independently by the standard Gaussian $N_{0,1}$.

B. Let G be the graph whose vertices are the points in (A) and where there is an arc from U to V if $d(U,V) < D$.

Then what is the probability that G is a connected graph?

Draw a plot of the probability vs. D for $N = 100$, over a range of value in which D goes from close to 0 to close to 1.

Draw a plot of the probability vs. N for $D = 0.1$ for $N = 2$ to a large enough value such that the probability is near 1.

Chapter 13

Information and Entropy

The two central concepts in information theory are the *information* of an event and the *entropy* of a random variable.

13.1 Information

The *information* of a probabilistic event E, denoted "$\mathrm{Inf}(E)$" measures the amount of information that you gain when you learn E, starting from scratch (i.e. from some presumed body of background knowledge). $\mathrm{Inf}(E)$ is measured in number of bits. As in probabilistic notation, "E, F' represents the event that both E and F are true; thus $\mathrm{Inf}(E, F)$ is the information gained by learning both E and F. The conditional information $\mathrm{Inf}(E|F)$ is the amount of information that you gain if you learn E after you have already learned F. Therefore $\mathrm{Inf}(E|F) = \mathrm{Inf}(E, F) - \mathrm{Inf}(F)$.

The information of E is related to its probability: $P(E) = 2^{-\mathrm{Inf}(E)} = 1/2^{\mathrm{Inf}(E)}$ or equivalently $\mathrm{Inf}(E) = -\log(P(E)) = \log(1/P(E))$. Likewise $\mathrm{Inf}(E|F) = -\log(P(E|F))$. (Throughout this chapter, $\log(x)$ means $\log_2(x)$.) Note that, since $P(E) \leq 1$, $\log(P(E)) \leq 0$, so $\mathrm{Inf}(E) \geq 0$; finding out the outcome of an event never constitutes a loss of information.

The intuition here is this: Suppose you have k independent events, each of which has probability $1/2$. Then, clearly, communicating the outcome of all these events requires k bits; thus, the sequence of k outcomes constitutes k bits of information. The probability of any particular sequence of outcomes is 2^{-k}. So for a random string S of k bits, $P(S) = 2^{-\mathrm{Inf}(S)}$ and $\mathrm{Inf}(S) = -\log(P(S))$. The natural generalization is that, for any event E, $\mathrm{Inf}(E) = -\log(P(E))$.

That last step may seem like a leap. We can elaborate it as follows: Let us suppose that the information function $\mathrm{Inf}(E)$ satisfies the following properties:

1. If E is an event of probability $1/2$, then $\mathrm{Inf}(E) = 1$ bit.
2. If $P(E) = P(F)$ then $\mathrm{Inf}(E) = \mathrm{Inf}(F)$. That is, the information of an event is purely a function of its probability.
3. $\mathrm{Inf}(E|F) = \mathrm{Inf}(E, F) - \mathrm{Inf}(F)$, as discussed above.
4. If E and F are independent events then $\mathrm{Inf}(E|F) = \mathrm{Inf}(E)$. The argument is as follows: If E and F are independent then knowing F gives you no information about E. Therefore, learning E after you know F gives you as much new information as learning E before you learned F.

5. The entropy is a continuous function of the probability distribution.

Given these five premises, one can prove that $\mathrm{Inf}(E) = -\log(P(E))$.

Proof: By premises (3) and (4), if E and F are independent, then $\mathrm{Inf}(E,F) = \mathrm{Inf}(F) + \mathrm{Inf}(E|F) = \mathrm{Inf}(F) + \mathrm{Inf}(E)$.

Let k be a large number. Let $F_1 \ldots F_k$ be independent events each of probability $2^{-1/k}$. Then $P(F_1, \ldots, F_k) = 1/2$ so $\mathrm{Inf}(F_1, \ldots, F_k) = 1$. But then
$1 = \mathrm{Inf}(F_1, \ldots, F_k) =$ (since they are independent)
$\mathrm{Inf}(F_1) + \ldots + \mathrm{Inf}(F_k) =$ (since they all have equal probability)
$k \cdot \mathrm{Inf}(F_1)$
so $\mathrm{Inf}(F_1) = 1/k$. Now let E be any event and let $q = \lfloor k \cdot -\log(P(E)) \rfloor$, so $\log(P(E)) \approx -q/k$.
Then $P(F_1, \ldots, F_q) = 2^{-q/k} \approx 2^{\log(P(E))} = P(E)$.
By the continuity premise (4) above, $\mathrm{Inf}(P(E)) \approx \mathrm{Inf}(F_1, \ldots, F_q) = q/k \approx -\log(P(E))$.
In the limit as k goes to infinity, the approximation converges to an equality. ∎

If you are still not convinced, we will give another argument below at the end of section 13.4.

For convenient reference, we will restate the above additivity properties of information as a theorem:

Theorem 13.1.

A. For any two events E and F, $\mathrm{Inf}(E,F) = \mathrm{Inf}(F) + \mathrm{Inf}(E|F)$

B. If E and F are independent, then $\mathrm{Inf}(E,F) = \mathrm{Inf}(E) + \mathrm{Inf}(F)$.

C. If $E_1 \ldots E_k$ are independent and have the same distribution, then $\mathrm{Inf}(E_1 \ldots E_k) = k \cdot \mathrm{Inf}(E_1)$.

Note that each of these is just the logarithm of the corresponding rule for probabilities:

A. $P(E,F) = P(F) \cdot P(E|F)$.
B. If E and F are independent then $P(E,F) = P(E) \cdot P(F)$.
C. If $E_1 \ldots E_k$ are independent and identically distributed then $P(E1 \ldots E_k) = (P(E_1))^k$.

13.2 Entropy

The *entropy* of random variable X, denoted $\mathrm{Ent}(X)$, is the expected value of its information: $\mathrm{Ent}(X) = \mathrm{Exp}(\mathrm{Inf}(X))$. Thus if X has distribution $\langle p_1, p_2 \ldots p_k \rangle$, then

$$\mathrm{Ent}(X) = -(p_1 \log(p_1) + \ldots + p_k \log(p_k))$$

By convention, if $p_i = 0$ we will take $p_i \log(p_i)$ to be 0.

Since the entropy only depends on the probability distribution, it is common to write $\mathrm{Ent}(p_1 \ldots p_k) = -(p_1 \log(p_1) + \ldots + p_k \log(p_k))$, the entropy of a random variable with distribution $\langle p_1 \ldots p_k \rangle$.

If X is a Boolean variable, with $P(X = t) = p$ and $P(X = f) = 1 - p$ then $\mathrm{Ent}(X) = \mathrm{Ent}(p, 1-p) = -(p \log(p) + (1-p) \log(1-p))$. This is shown as a function of p in figure 13.1. For $p = 0$ and $p = 1$ we have $\mathrm{Ent}(X) = 0$. (If $p = 0$, then the event $X = t$ has infinite information but zero chance of occurring; and the event $X = f$ will certainly occur, but carries zero information.) The function reaches a maximum of 1 at $p = 1/2$. If $p = \epsilon$ or $p = 1 - \epsilon$ where ϵ is small, then $\mathrm{Ent}(X) \approx -\epsilon \log \epsilon$.

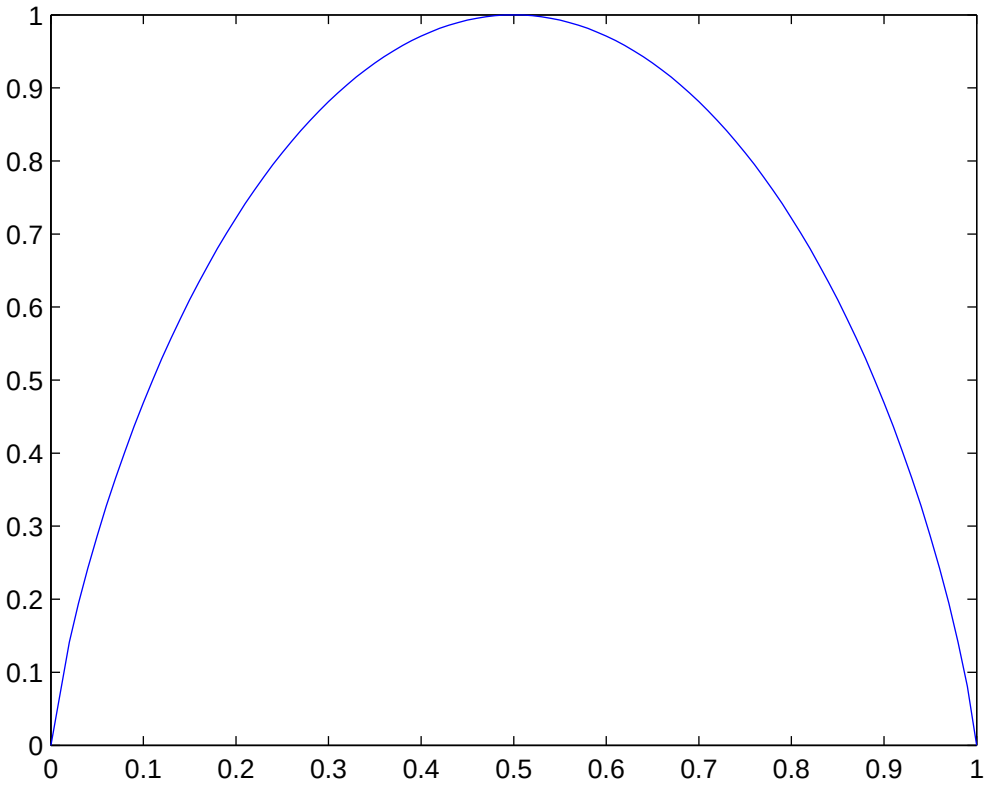


Figure 13.1: Entropy function

If X is a random variable with k values, each of probability $1/k$ then $\text{Ent}(X) = \text{Ent}(1/k \ldots 1/k) = \log(k)$. It is a fact that we will discuss further in section 13.6 that if Y is any random variable with k values then $\text{Ent}(Y) \leq \text{Ent}(X) = \log(k)$

13.3 Conditional Entropy and Mutual Information

Let E be an event and let X be a random variable. The *entropy of X given E* is the entropy of X once you know E,

$$\text{Ent}(X|E) = -\sum_x P(X = x|E) \log(P(X = x|E))$$

We can consider "$X|E$" to be a random variable over the range of X defined by the equation that $P((X|E) = x) = P(X = x|E)$. In that case $\text{Ent}(X|E)$ is simply entropy of the random variable $X|E$.

Let Y be a second random variable. The *conditional entropy of X given Y* is the expected value, taken over all the possible values y of Y of [the conditional entropy of X given $Y = y$].

$$\text{CEnt}(X|Y) = \sum_y P(Y = y) \cdot \text{Ent}(X|Y = y) = -\sum_{x,y} P(Y = y) \cdot P(X = x|Y = y) \log(P(X = x|Y = y))$$

That is: Imagine that you currently don't know the value of either X or Y, but you are about to find out Y. The conditional entropy $\text{CEnt}(X|Y)$ measures what you can expect that the entropy of X will be, on average, after you find out Y.

Note that the entropy conditioned on an event $\text{Ent}(X|E)$ is indeed an entropy of the random variable $X|E$. The "conditional entropy" of variable X conditioned on variable Y, $\text{CEnt}(X|Y)$ is not actually the entropy of any random variable, which is why we use a different symbol.

Theorem 13.2. *For any two random variables X and Y, $\text{Ent}(X, Y) = \text{Ent}(Y) + \text{CEnt}(X|Y)$. If X and Y are independent, $\text{CEnt}(X|Y) = \text{Ent}(X)$ and $\text{Ent}(X, Y) = \text{Ent}(X) + \text{Ent}(Y)$.*

Proof: The first statement follows from theorem 13.1 and the additivity of expected value. The second follows from the definition of conditional entropy. ∎

Example 13.1: Suppose that X has two values $\{f, t\}$ and $P(X = f) = P(X = t) = 1/2$. Y is independent of X; it has values $\{r, w, b\}$ and $P(Y = r) = 1/2$; $P(Y = w) = 1/4$ and $P(Y = b) = 1/4$. Then

$$\text{Ent}(X) = -(1/2 \cdot \log(1/2) + 1/2 \cdot \log(1/2)) = 1.$$

$$\text{Ent}(Y) = -(1/2 \cdot \log(1/2) + 1/4 \cdot \log(1/4) + 1/4 \cdot \log(1/4)) = 3/2.$$

The joint distribution of X, Y is

$$\begin{array}{lll} P(X = f, Y = r) = 1/4. & P(X = f, Y = w) = 1/8. & P(X = f, Y = b) = 1/8. \\ P(X = t, Y = r) = 1/4. & P(X = t, Y = w) = 1/8. & P(X = t, Y = b) = 1/8. \end{array}$$

So $\text{Ent}(X, Y) =$
$-(1/4 \cdot \log(1/4) + 1/8 \cdot \log(1/8) + 1/8 \cdot \log(1/8) + 1/4 \cdot \log(1/4) + 1/8 \cdot \log(1/8) + 1/8 \cdot \log(1/8)) =$
$5/2 = \text{Ent}(X) + \text{Ent}(Y)$

Example 13.2: Let W and Z be random variables with the following joint distribution.

$$P(W=f,Z=r)=0.4. \quad P(W=f,Z=w)=0.05. \quad P(W=f,Z=b)=0.05.$$
$$P(W=t,Z=r)=0.1 \quad P(W=t,Z=w)=0.1 \quad P(W=t,Z=b)=0.3$$

Thus W and Z are not independent; if $W=f$, then probably $Z=r$, and if $W=t$ then probably $Z=b$.

$$P(Z=r|W=f)=0.8 \quad P(Z=w|W=f)=0.1 \quad P(Z=b|W=f)=0.1$$
$$P(Z=r|W=t)=0.2 \quad P(Z=w|W=t)=0.2 \quad P(Z=b|W=t)=0.6$$

So we have:

$\mathrm{Ent}(W)=\mathrm{Ent}(1/2,1/2)=1.$
$\mathrm{Ent}(Z|W=f)=\mathrm{Ent}(0.8,0.1,0.1)=0.9219.$
$\mathrm{Ent}(Z|W=t)=\mathrm{Ent}(0.2,0.2,0.6)=1.3710.$
$\mathrm{CEnt}(Z|W)=$
$P(W=f)\cdot\mathrm{Ent}(Z|W=f)+P(W=t)\cdot\mathrm{Ent}(Z|W=t)=$
$0.5\cdot 0.9219+0.5\cdot 1.3710=1.1464$
$\mathrm{Ent}(W,Z)=\mathrm{Ent}(0.4,0.05,0.05,0.1,0.1,0.3)=2.1464.$

Note that $\mathrm{Ent}(W,Z)=\mathrm{Ent}(W)+\mathrm{CEnt}(Z|W)$.

It is a remarkable fact that the conditional entropy is always less than or equal to the entropy.

Theorem 13.3. *For any two random variables X and Y, $\mathrm{CEnt}(X|Y)\leq\mathrm{Ent}(X)$, with equality holding if and only if X and Y are independent.*

We omit the proof of theorem 13.3. What this theorem means is that on average, finding out Y decreases your uncertainty about X, unless the two are independent, in which case it leaves the uncertainty unchanged. It is certainly true that finding out a particular *event* can increase your uncertainty. If you see that the clock reads 2:45, then your entropy on the time of day is low; if you then observe that the clock is stopped, then the entropy goes way up again. But that can only happen because it was originally unlikely that the clock would be stopped; if you had known from the first that the clock might well be stopped, then your original probability distribution on the time would have been much smoother and the original entropy much higher. In either case, finding out the reverse fact, that the clock is running, will lower your entropy on the time; if you had originally thought it likely that the clock might be stopped, finding out that it is running will lower the entropy by a good deal. What theorem 13.3 states is that, on average, finding out whether or not the clock is running cannot increase your entropy on the time of day, and it can only fail to decrease your entropy if the random variables "Status of Clock" and "Time of Day" are independent (which they probably are).

Theorem 13.2 has the following interesting consequence. We have $\mathrm{Ent}(X,Y)=\mathrm{Ent}(Y)+\mathrm{CEnt}(X|Y)$. By symmetry, it is equally true that $\mathrm{Ent}(X,Y)=\mathrm{Ent}(X)+\mathrm{CEnt}(Y|X)$. It follows, therefore that $\mathrm{Ent}(Y)-\mathrm{CEnt}(Y|X)=\mathrm{Ent}(X)-\mathrm{CEnt}(X|Y)$. This quantity is known as the *mutual information* of X and Y, denoted $\mathrm{MInf}(X,Y)$. Since entropy is a measure of uncertainty, this measures how much less uncertain you are about Y once you have learned X; in other words, how much (in bits) you learn about Y when you find out the value of X. The above equation states that this is equal to the amount you learn about X when you find out the value of Y. By theorem 13.3 this is always non-negative and it is zero only if X and Y are independent. In example 13.2, we have

$\mathrm{Ent}(Z)=\mathrm{Ent}(0.5,0.15,0.35)=1.4406)$ so
$\mathrm{MInf}(W,Z)=\mathrm{Ent}(Z)-\mathrm{CEnt}(Z|W)=1.4406-1.1464=0.2942.$

So if you originally know the distribution of Z and then you find out the value of W, you have gained 0.2942 bits of information about the value of Z.

13.4 Coding

The entropy of a probability distribution is a critical number in calculating how efficiently a string generated by a random process can be transmitted. This problem and other problems relating to the transmission of information were indeed the original motivation for the invention of information theory by Claude Shannon in the late 1940's and early 1950's.

We will address the problem of encoding a finite string of characters as a string of bits. We assume that the character string is drawn from a finite alphabet, denoted $\mathcal{A}$.

Definition 13.1. *Let $\mathcal{A}$ be a finite alphabet. Then the set of all strings of characters in $\mathcal{A}$ of length exactly n will be denoted $\mathcal{A}^n$. The set of all finite strings will be denoted $\mathcal{A}^\omega$*

In particular, we will be interested in the alphabet of bits $\{0, 1\}$, which we will denote $\mathcal{B}$.

Definition 13.2. *Let $\mathcal{A}$ be an alphabet. A* coding scheme for $\mathcal{A}$ *is an injection from $\mathcal{A}^\omega$ into $\mathcal{B}^\omega$.*

That is, a coding scheme $\Gamma(s)$ is a function that maps every string over $\mathcal{A}$ in an unambiguous way; if $x, y \in \mathcal{A}$ and $x \neq y$ then $\Gamma(x) \neq \Gamma(y)$.

For any string s, we will denote the length of s as $|s|$.

Suppose that we need to communicate very long strings over $\mathcal{A}$, that are generated by choosing each character in the string independently, according to a distribution given by random variable X. We want to design a coding scheme Γ that encodes these strings efficiently, in terms of the lengths of the bit strings output. We measure the efficiency of Γ by fixing a large value of n, asking what is the expected number of bits in $\Gamma(s)$ where s is a string of length n generated by this random process, and dividing that expected number by n. We then let n go to infinity; this is the asymptotic efficiency of Γ, denoted $\mathrm{BpC}(\Gamma, X)$ (Bits per Character). (If the limit as n goes to infinity does not exist, then $\mathrm{BpC}(\Gamma, X)$ is undefined,)

Definition 13.3. *Let X be a random variable over $\mathcal{A}$. Let $X_1 \ldots X_n$ be independent random variables with the same distribution as X. Then X^n will denote the joint distribution of $X_1 \ldots X_n$.*

Thus X^n is a random variable over $\mathcal{A}^n$ corresponding to choosing each character in the string independently according to X.

Definition 13.4. *Let X be a probability distribution over $\mathcal{A}$ and let Γ be a coding scheme for X. The* bit per character ratio *for Γ over X is defined as follows:*

$$\mathrm{BpC}(\Gamma, X) = \lim_{n \to \infty} \mathrm{Exp}(|\Gamma(X^n)|)/n$$

assuming that this limit exists.

Example 13.3: Let $\mathcal{A} = \{a, b, c, d\}$ and let X have the distribution

$P(X = a) = 3/4$
$P(X = b) = 1/8$
$P(X = c) = 1/16$
$P(X = d) = 1/16$

Let Γ_1 be defined as follows: Do a character-by-character encoding where $a \to 00$, $b \to 01$, $c \to 10$, and $d \to 11$. For example $\Gamma_1(\text{“aacaaadbaab”}) = \text{“00001000000011010000001”}$ For readability, I will

henceforth add commas which aren't actually in the bit string; thus, the previous string will be written "00,00,10,00,00,00,11,01,00,00,01". Then for any string $s \in \mathcal{A}^\omega$, $|\Gamma_1(s)| = 2|s|$. In particular for any $s \in \mathcal{A}^n$, $|\Gamma_1(s)| = 2n$. Therefore $\mathrm{BpC}(\Gamma_1, X) = 2$; this holds for any distribution X.

Example 13.4: Let $\mathcal{A}$ and X be as in example 13.3. Let Γ_2 be defined as follows: Do a character-by-character encoding where $a \to 0$, $b \to 10$, $c \to 110$ $d \to 111$. For example Γ_2("aacaaadbaab") = "0,0,110,0,0,0,111,10,0,0,10".

Consider forming a n-character string in $\mathcal{A}^n$, and let $X_1, X_2 \ldots X_n$ be random variables where the value of X_i is the ith character in the string. Then $|\Gamma_2(X^n)| = |\Gamma_2(X_1)| + \ldots + |\Gamma_2(X_n)|$ so $\mathrm{Exp}(|\Gamma_2(X^n|) = \mathrm{Exp}(|\Gamma_2(X_1)|) + \ldots + \mathrm{Exp}(|\Gamma_2(X_n)|) = n \cdot \mathrm{Exp}(|\Gamma_2(X)|)$, since all the X_i have the same distribution as X. But

$\mathrm{Exp}(|\Gamma(X)|) =$
$P(X = `a') \cdot |\Gamma_2(`a')| + P(X = `b') \cdot |\Gamma_2(`b')| + P(X = `c') \cdot |\Gamma_2(`c')| + P(X = `d') \cdot |\Gamma_2(`d')| =$
$(3/4) \cdot 1 + (1/8) \cdot 2 + (1/16) \cdot 3 + (1/16) \cdot 3 = 11/8 = 1.375.$

Therefore $\mathrm{Exp}(|\Gamma_2(X^n|) = n \cdot \mathrm{Exp}(|\Gamma_2(X)|) = 1.375n$ so $\mathrm{BpC}(\Gamma_2, X) = 1.375$. Note that this is substantially smaller than $\mathrm{BpC}(\Gamma_1, X) = 2$.

It is not obvious on the face of it that Γ_2 is a coding scheme at all, because it is not obvious that there could not be two alphabetic strings with the same encoding (once the commas are removed). However, one can prove that encodings are unique because this scheme is *prefix free*; that is, no code for one character is a prefix for another. That being the case, the bit string can be read left to right, "peeling off" the code for each character at a time. For example, to decode the string "0100111101100" we observe that

> The first '0' is a code for 'a' and does not start the code for any other character.
> The '1' at index 2 is not in itself a code for anything. The '10' at index 2-3 is a code for 'b' and does not start the code for any other character.
> The '0' at index 4 is a code for 'a' and does not start the code for any other character.
> The '1' at index 5 and the '11' at index 5-6 are not in themselves codes for anything.
> The '111' at indices 5-7 is the code for 'd'.

Continuing on in this way, one can recover the entire string.

We can generalize this observation in the following definition and theorem:

Definition 13.5. *A set S of bit strings is* prefix-free *if no element in S is a prefix of any other element.*

A prefix-free code corresponds to a set of leaves in a binary tree (figure 13.2, 13.3.)

Definition 13.6. *A* character code *over $\mathcal{A}$ is an injection from $\mathcal{A}$ to $\mathcal{B}^\omega$*

A character code Γ over $\mathcal{A}$ is prefix-free *if $\Gamma(\mathcal{A})$ is a prefix-free set.*

Definition 13.7. *A function Γ from $\mathcal{A}^\omega$ is a* simple code *if*

- *Γ is a character code over $\mathcal{A}$;*
- *for any string $s = \langle s[1] \ldots s[k] \rangle$, $\Gamma(s)$ is the concatenation of $\Gamma(s[1]) \ldots \Gamma(s[k])$.*

Theorem 13.4. *If Γ is a simple code which is prefix-free over $\mathcal{A}$, then Γ is an unambiguous coding scheme over $\mathcal{A}^\omega$*

Proof: Using the left-to-right decoding method described above, it is clear that any bit string can be decoded in at most one way.

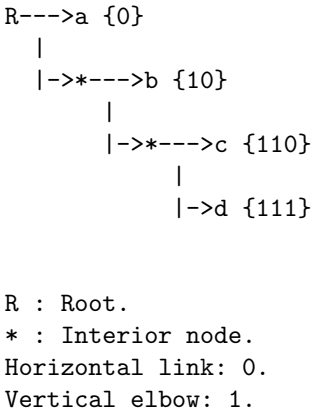


Figure 13.2: Binary tree for code Γ_2

Example 13.5: Let $\mathcal{A}$ and X be as in example 13.3. Let $\Gamma_3(s)$ be defined as follows: Break s up into two-character blocks; if s is odd, there will be a final one-character block. Do the following block-by-block encoding: (The corresponding binary tree is shown in figure 13.3.)

$aa \to 0$	$ab \to 100$	$ac \to 1100$	$ad \to 1101$
$ba \to 101$	$bb \to 1111100$	$bc \to 11111010$	$bd \to 11111100$
$ca \to 1110$	$cb \to 11111011$	$cc \to 111111100$	$cd \to 111111101$
$da \to 11110$	$db \to 11111101$	$dc \to 111111110$	$dd \to 1111111110$
Final $a \to 111111111100$	Final $b \to 111111111101$	Final $c \to 111111111110$	Final $d \to 111111111111$

In a string of length n there will be $\lfloor n/2 \rfloor$ blocks of length 2 and possibly 1 block of length 1. We can ignore the final block, in the limit as $n \to \infty$. The expected total length of the non-final blocks is

$(n/2) \cdot [P(`aa') \cdot |\Gamma(`aa')| + P(`ab') \cdot |\Gamma(`ab')| + \ldots + P(`dd') \cdot |\Gamma(`dd')| \,] =$
$(n/2)[(9/16) \cdot 1 + (3/32) \cdot 3 + \ldots + (1/256) \cdot 10] =$ (if you work it out) $1.2129n$

So $\mathrm{BpC}(\Gamma_3) = 1.2129$. Note that we have achieved a still greater compression.

How efficient can we make these codes? The answer, as we shall prove below, is that we can get codes whose BpC is arbitrarily close to the entropy, and that we cannot do better than the entropy. In examples 13.3 — 13.5, the entropy is $-((3/4)\log(3/4)+(1/8)\log(1/8)+(1/16)\log(1/16)+(1/16)\log(1/16) = 1.1863$, so the code in example 13.5 is within 2.5% of optimal.

Examples 13.4 and 13.5 above illustrate two techniques used to make the naive code of example 13.3 more efficient. First, we assign shorter codes to more common characters and longer codes to less common ones, lowering the overall average. Second, we group the characters into blocks; this allows us to carry out the first technique with more delicate discrimination.

We now prove three theorems that show the effectiveness of these techniques. Theorem 13.5 states that by applying the first technique you can get a simple prefix-free code with a BpC which is at most the entropy plus 1. Theorem 13.6 states that by applying both techniques you can get a non-simple code with a BpC that is arbitrarily close to the entropy. Theorem 13.8 states that no coding scheme of any kind can have a BpC which is less than the entropy.

Theorem 13.5. *Let $\mathcal{A}$ be an alphabet and let X be a random variable over $\mathcal{A}$. There exists a simple code Γ for $\mathcal{A}$ such that* $\mathrm{BpC}(\Gamma, X) \leq \mathrm{Ent}(X) + 1$.

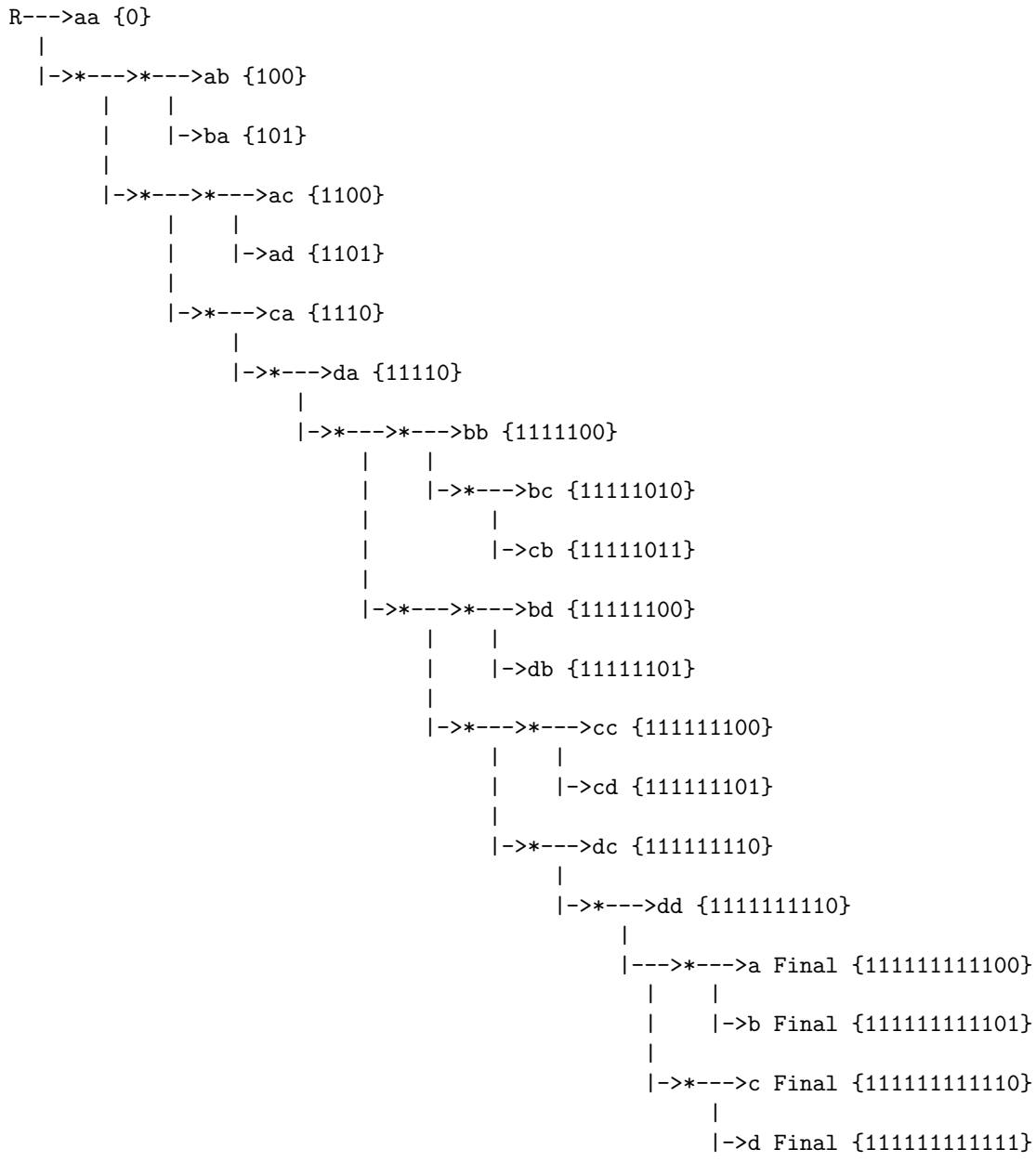


Figure 13.3: Binary tree for code Γ_3

Proof: We will give an algorithm that constructs such a code. As in figures 13.2 and 13.3, we assign a leaf of a binary tree to each character in $\mathcal{A}$. The assignments are carried out in descending order of probability. Each character α_i is placed at depth $\lceil -\log(P(X = \alpha_i)) \rceil$ immediately to the right of the previous character, so the leaves of the tree slant downward to the right.

The algorithm is as follows:

function ConstructCode(**in:** $\mathcal{A}$: Alphabet; P: probability distribution)
return: code for $\mathcal{A}$.

{ $k \leftarrow |\mathcal{A}|$;
$\langle \alpha_1 \ldots \alpha_k \rangle \leftarrow$ $\mathcal{A}$ sorted in descending order of $P(\alpha)$.
$h = \lceil -\log(P(\alpha_k)) \rceil$;
Construct a binary tree of depth h. Label each left arc '0' and each right arc '1'.
for $(i \leftarrow 1 \ldots k)$ {
$L_i \leftarrow \lceil -\log(P(\alpha_i)) \rceil$;
$N \leftarrow$ the leftmost node of depth L_i that is neither marked or pruned;
mark N as "in use";
assign to α_i the code that is the sequence of arc labels from the root to N;
prune the subtree under N;
}
return the assignment of codes to the α_i;
}

We can analyze the behavior of this algorithm in terms of how the node that are assigned cover the "original" leaves; that is, the leaves of the starting uniform tree of depth h. Note that:

- N_i covers a subtree with 2^{h-L_i} original leaves.
- Since L_i increases with i, for $j < i$, the number of original leaves pruned on the jth step, 2^{h-L_j} is a integer multiple of 2^{h-L_i}.
- Therefore, the total number of original leaves that have been labeled or pruned before the start of the ith iteration of step 4 is a multiple of 2^{h-L_i}.
- Therefore, in the course of executing step 4, the original leaves are labelled or pruned in consecutive, left-to-right order.
- The fraction of original leaves that are covered on the ith step is 2^{-L_i}. Since $\sum_i 2^{-L_i} \leq \sum_i p_i = 1$, we do not run out of original leaves.

Let Γ be the code corresponding to this labelling. Note that for every i, $|\Gamma(\alpha_i)| = \lceil -\log(p_i) \rceil < -\log(p_i) + 1$. Therefore,

$$\mathrm{BpC}(\Gamma, X) = \mathrm{Exp}(|\Gamma(X)|) = \sum_i p_i |\Gamma(\alpha_i)| < \sum_i p_i(-\log(p_i) + 1) = \mathrm{Ent}(X) + 1$$

∎

Example 13.6 Suppose that $\mathcal{A} = \{a, b, c, d, e\}$ and $p_1 = 0.3$; $p_2 = 0.27$; $p_3 = 0.21$; $p_4 = 0.17$, and $p_5 = 0.05$. Then $L_1 = 2, L_2 = 2, L_3 = 3, L_4 = 3, L_5 = 5$. The tree is shown in figure 13.4. The code Γ_4 is

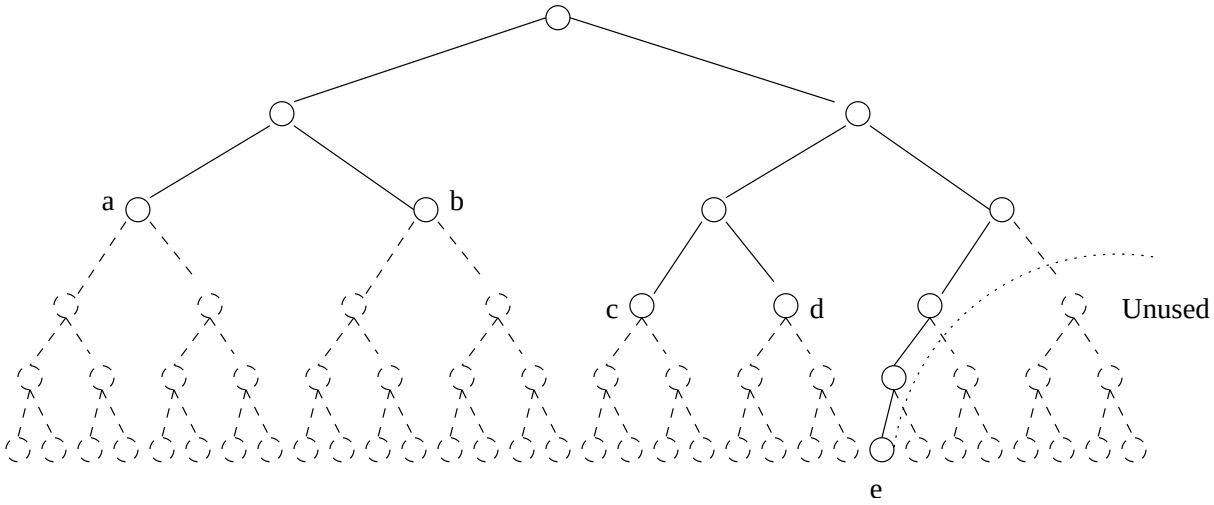


Figure 13.4: Example 13.6

$\Gamma_4(a) = 00$.
$\Gamma_4(b) = 01$.
$\Gamma_4(c) = 100$.
$\Gamma_4(d) = 101$.
$\Gamma_4(e) = 11000$.

$\text{BpC}(\Gamma_4, X) = \text{Exp}(|\Gamma_4(X)|) = 2.53$. $\text{Ent}(X) = 2.155$

Clearly this code is nothing like optimal, but it satisfies the theorem. We will present an algorithm for generating the optimal code in section 13.4.1.

Definition 13.8. *Let $m \geq 1$. Let $\mathcal{A}^{\leq m}$ be the set of all strings of $\mathcal{A}$ of length at most m. An* m-block *code over alphabet $\mathcal{A}$ is an injection from $\mathcal{A}^{\leq m}$ to $\mathcal{B}^\omega$; that is, a code for every block of characters of size at most m. In particular, a character code is a 1-block code.*

Γ *is an* m-simple code *if*

- Γ *restricted to $\mathcal{A}^{\leq m}$ is an m-block code;*
- *If s is a string of length greater than m, then $\Gamma(s)$ is obtained by breaking Γ into blocks of length m starting at the left, leaving a final block of length $\leq m$, and then concatenating the output of Γ on each of the blocks.*

An m-simple code Γ is prefix-free *if $\Gamma(\mathcal{A}^{\leq m})$ is a prefix-free set.*

Theorem 13.6. *Let $\mathcal{A}$ be an alphabet and let X be a random variable over $\mathcal{A}$. Let $\epsilon > 0$, and let $m > 1/\epsilon$. There exists a prefix-free m-simple coding scheme Γ for $\mathcal{A}$ such that* $\text{BpC}(\Gamma, X) \leq \text{Ent}(X) + \epsilon$.

Proof: Consider $\mathcal{A}^m$ to be a "super-alphabet" of character blocks of length m, and consider the distribution X^m over $\mathcal{A}$. Then by theorem 13.5, there exists a simple code Γ for $\mathcal{A}$ such that $\text{BpC}(\Gamma, X^m) \leq \text{Ent}(X^m) + 1$. (The encoding of the final blocks does not matter since there is only one of these per string, and hence they add a negligible length as length of the string goes to infinity.) However, since the "characters" of $\mathcal{A}^m$ are blocks of m characters of $\mathcal{A}$, we have $\text{BpC}(\Gamma, X^m) =$

$m \cdot \mathrm{BpC}(\Gamma, X)$. By theorem 13.1.C $\mathrm{Ent}(X^m) = m \cdot \mathrm{Ent}(X)$, so $m \cdot \mathrm{BpC}(\Gamma, X) \leq m \cdot \mathrm{Ent}(X) + 1$. Dividing through by m we get is $\mathrm{BpC}(\Gamma, X) \leq \mathrm{Ent}(X) + 1/m < \mathrm{Ent}(X) + \epsilon$. ∎

We will not give a rigorous proof of theorem 13.8, that any coding scheme has a BpC of at least the entropy. Rather, we will give an approximate argument, and then wave our hands to indicate how the holes in the argument are fixed. First, we prove the following lemma:

Lemma 13.7. *Let D be a domain of size n, and let random variable X be uniformly distributed over $\mathcal{A}$. Let Γ be an injection from D to $\mathcal{B}^\omega$ Then* $\mathrm{Exp}(\Gamma(X)) \geq \log(n) - 3$.

Note that we don't require that Γ is a prefix-free code, or that it will be an unambiguous code once you string characters and codes together. The only property we require of Γ is that it is one-to-one over $\mathcal{A}$. Also, with a more careful analysis one can improve the bound in this lemma, but this is sufficient for our purposes.

Proof: Clearly, the shortest average is attained with Γ uses uses all possible short bit strings. Note that there are 2 bit strings of length 1, 4 of length 2, 8 of length 3 and so on. Therefore, the number of strings of length at most k is $2 + 4 + \ldots + 2^k = 2^{k+1} - 2$. To get n different strings, therefore, we must have $2^{k+1} - 2 \geq n$ so $k \geq \log(n+2) - 1 > \log(n) - 1$. Let us ignore the strings of length k. Considering only the strings of length less than k, their total length is $(\sum_{i=1}^{k-1} i \cdot 2^i) = (k-2) \cdot 2^k + 2$ so their average length is $((k-2) \cdot 2^k + 2)/(2^k - 2) > k - 2 > \log(n) - 3$. ∎

Theorem 13.8. *(Shannon's theorem) Let $\mathcal{A}$ be an alphabet and let X be a random variable over $\mathcal{A}$. Let Γ be a coding scheme for $\mathcal{A}$. Then* $\mathrm{BpC}(\Gamma, X) \geq \mathrm{Ent}(X)$.

Argument: Let $\alpha_1, \alpha_2 \ldots \alpha_k$ be the characters of $\mathcal{A}$ and let $\langle p_1, p_2 \ldots p_k \rangle$ be the distribution of X.

Let n be large, and consider the distribution X^n. With very high probability, a string of n characters chosen according to X^n has approximately $p_1 \cdot n$ occurrences of α_1, $p_2 \cdot n$ occurrences of α_2, $\ldots p_k \cdot n$ occurrences of α_k. Assume for simplicity that $p_i \cdot n$ is an integer for all i.

Let us imagine, for the moment, that the only strings we have to worry about are those that have *exactly* $n \cdot p_i$ occurrences of α_i. That is: Let Y be a random variable which is uniformly distributed over those strings with *exactly* $n \cdot p_i$ occurrences of α_i. All of these strings are equally probable. According to the partition formula, discussed in section 8.3, the number of such strings Q is given by the formula

$$Q = C\left(\begin{array}{c} n \\ n \cdot p_1, n \cdot p_2 \ldots n \cdot p_k \end{array} \right) = \frac{n!}{(n \cdot p_1)! \cdot (n \cdot p_2)! \ldots (n \cdot p_k)!}$$

Therefore, by lemma 13.7, for any coding scheme Γ, $\mathrm{Exp}(|\Gamma(Y)|) > \log(Q) - 3$. Using a little algebra (details below) we can show that $\log(Q) \approx n \cdot \mathrm{Ent}(p_1 \ldots p_k)$. Each string of Y is of course n characters of X. Therefore, if X gave rise to Y, then we could say that $\mathrm{BpC}(\Gamma(X)) \geq \lim_{n \to \infty} \mathrm{Exp}(|\Gamma(Y)|)/n = \mathrm{Ent}(p_1 \ldots p_k)$, since the $3/n$ term becomes negligible.

Of course, the distribution over strings of length n that X actually generates is not Y; it is the multinomial distribution. However, the differences turn out not to matter to this calculation. To do the analysis it is convenient to divide strings into two categories; those that are "close to" Y – i.e. within some number of standard deviations — and those that are far from Y. We can then note the following gaps in our argument.

- $n \cdot p_i$ may not be an integer. That is purely nuisance value; one can round to an integer with negligible effect on the computation
- Some of the strings far from Y are, individually, much more probable than the strings in Y; for instance, the string that consists entirely of the most probable symbol repeated n times.

But the total probability that X will generate *any* string far from Y is so small that they can be collectively ignored.

- There are lots of strings close to Y that are don't exactly fit with Y; in fact since we can vary by $\sqrt{n}$ independently in $k-1$ dimensions, there are on the order of $n^{(k-1)/2}$ times as many strings close to Y as in Y. But increasing the number of strings only makes it harder to keep the BpC small. It may seem surprising in the opposite direction, that multiplying the number of options by this large factor does not force an increase in the BpC, but the point is, when you take the logarithm, this just amounts to adding a term of the form $(k-1)\log(n)/2$, which is negligible as compared to n.
- Some of the strings close to Y are in fact more probable than the strings in Y (those that have more of the popular characters and fewer of the unpopular characters), and the total probabilities of these is non-negligible. But they are actually not enough more probable to affect the calculation.

These arguments can be made rigorous, but doing so involves more calculation than is worthwhile here.

Let us return to the problem of computing $\log(Q)$:

$$\log(Q) = \log\left(\frac{n!}{(n\cdot p_1)!\cdot(n\cdot p_2)!\ldots(n\cdot p_k)!}\right) = \log(n!) - [\log((n\cdot p_1)!) + \log((n\cdot p_2)!) + \log((n\cdot p_k)!)]$$

By Stirling's formula, $\ln(n!) = n\ln(n) - n + O(\ln(n))$ so $\log(n!) = n\log(n) - n/\ln(2) + O(\log(n))$. So the above expression becomes

$$\log(Q) = n\log n - n/\ln(2) - [(np_1\log(np_1) - np_1/\ln(2)) + \ldots + (np_k\log(np_k) - np_k/\ln(2)] + O(\log(n)) =$$

$$n\log n - n/\ln(2) - np_1(\log n + \log p_1 - (n/\ln(2))p_1 + \ldots + np_k(\log n + \log p_k - (n/\ln(2))p_k + O(\log(n)$$

Using the fact the p_i add up to 1, the $n\log n$ terms cancel, the $n/\ln(2)$ terms cancel, and what remains is

$$\log(Q) = -n[p_1\log(p_1) + \ldots + p_k\log(p_k)] + O(\log(n)) = n\cdot\mathrm{Ent}(X) + O(\log(n))$$

∎

The key point about this argument is that the only assumption it makes about Γ is that Γ maps each string of characters to a unique bit string. Beyond that, it is just a counting argument; the argument is, essentially, that there are so many strings of length n with the right distribution, that you will need $n\cdot\mathrm{Ent}(p_1\ldots p_k)$ bits just to give each of these a different encoding.

These theorems support another argument in favor of measuring the information of E as $\log_2 P(E)$. If event E is one outcome of a random process P, and you need to communicate many long strings of outcomes of independent trials of P, then the best coding you can do will require, on average, $\log_2 P(E)$ bits for each occurrence of E. So it makes sense to say that E involves $\log_2 P(E)$ bits to be transmitted.

13.4.1 Huffman coding

The Huffman coding algorithm computes the optimal simple code — that is, the simple code with the smallest possible BpC — given a distribution over an alphabet. The algorithm constructs a

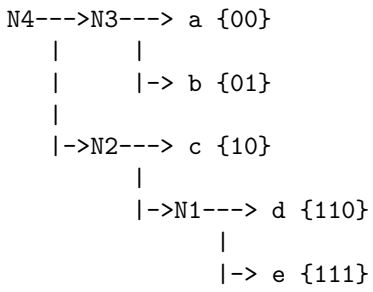


Figure 13.5: Huffman code

binary tree, comparable to figure 13.2, in which the leaves are the alphabetic characters and the code for a letter corresponds to the path to the letter from the root.

The Huffman coding algorithm builds the tree bottom up. At each iteration of the main loop, there is a forest of disjoint trees. Initially each character is in a tree by itself; at the end there is a single tree, labelled with a weight equal to its probability. At each iteration the two trees of minimum total weight become the two children of a new parent node; thus, the number of trees is reduced by one at each stage. The weight of the new tree is the sum of the weights of the children.

```
function T = Huffman(A: alphabet; P: distribution over A)
  for (each character u in A)
      create a leaf node for u labelled P(u);
  end
  S = the set of all leaf nodes;
  for I=1:size(A)-1
    [P,Q] = the two nodes in S with the smallest label
    create a new node N;
    make P and Q the two children of N;
    N.weight = P.weight + Q.weight;
    Add N to S and delete P and Q from S;
  end
end
```

Applying this algorithm to the distribution in example 13.6, we begin with five trees: characters a, b, c, d, e with weights 0.3, 0.27, 0.21, 0.17, 0.5. The algorithm proceeds through the following steps.

Make d and e children of $N1$ with weight 0.22.
Make c and $N1$ children of $N2$ with weight 0.43.
Make a and b children of $N3$ with weight 0.57.
Make $N2$ and $N3$ children of $N4$ with weight 1

The resultant tree is shown in figure 13.5.

For the proof of the correctness of the Huffman coding algorithm, see (Luenberger, 2006).

13.5 Entropy of numeric and continuous random variables

The entropy of a discrete numeric random variable is defined in the same way as above: $\text{Ent}(X) = \sum_v -P(X = v)\log(P(X = v))$. Note that this makes no use of the actual value v of X, just of the various values of the probabilities. As a consequence, it is a somewhat strange measure. For example, consider the following three random variables X, Y, Z.

$P(X = 0) = 1/2$. $P(X = 1) = 1/2$.
$P(Y = -0.01) = -1/4$. $P(Y = 0.01) = 1/4$. $P(Y = 1) = 1/2$.
$P(Z = 100) = 1/2$. $P(Z = 1000) = 1/2$.

Intuitively, X seems much more similar to Y than to Z, and on most measures, such as expected value and standard deviation, it is. However $\text{Ent}(X) = \text{Ent}(Z) = 1$ whereas $\text{Ent}(Y) = 3/2$.

As one would expect, the formula for the entropy of a continuous variable is obtained by replacing the probability by the probability density and summation by integration. If random variable X has p.d.f. $p(t)$ then

$$\text{Ent}(X) = \int_{-\infty}^{\infty} -p(t)\log(p(t))dt$$

Working out the definite integrals, one can show that, if X has the uniform distribution from l to $l + a$ then $\text{Ent}(X) = \log(a)$, which is very satisfying. One can also show that that if X has the normal distribution $N_{\mu,\sigma}$ then $\text{Ent}(X) = \log(\sigma) + (1/2)\log(2\pi e)$, which is less elegant, though it is remarkable that it is a closed-form expression at all.

Note that this can be negative; for instance, if $a < 1$ or $\sigma < 1/\sqrt{2\pi e}$. That seems odd; does finding out the value of this random variable constitute a *loss* of information? The answer is that we are not considering finding out the actual value, which would require infinite information. (Specifying all the digits of a real number is an infinite amount of information.) Rather, we are doing the following: In the discrete case, we are considering moving from knowing that $P(X = v) = p$ to knowing that $P(X = v) = 1$; measuring the change in information; and averaging that information change over all v weighted by $P(X = v)$. In the continuous case, we are considering moving from knowing that $\tilde{P}(X = v) = f(v)$ to $\tilde{P}(X = v) = 1$; measure the information change; and integrate that information change over all v weighted by $\tilde{P}(X = v)$. But if $\tilde{P}(X = v) > 1$, then indeed this constitutes a loss of information at v.

In general, if X is continuous random variable and c is a constant then $\text{Ent}(cX) = \log c + \text{Ent}(X)$. (The distribution of cX is c times wider and $1/c$ times the height of X, so the distribution is a lower probability density.)

See (Luenberger 2006 chap. 21) for further discussion of the entropy of continuous random variables.

13.6 The principle of maximum entropy

The entropy of a random variable X is the expected gain in information from finding out the value of X. However, in many cases it is more useful to think of it as a measure of *ignorance*;[1] it measures how much you *don't* know about the value of X if all you know is the distribution of X. This in turn suggests the following principle:

[1] However, the "stopped clock" example of section 13.2 illustrates that this view has to be taken with a grain of salt. It would be strange to say that finding out that the clock is stopped makes you more ignorant of the time; it just makes you aware that you were already ignorant of the time.

The Principle of Maximum Entropy.

> If you do not know the distribution of a random variable X but you have some constraints on it, then you should assume that you are as ignorant as possible of the value of X, and that therefore the true distribution is the one that maximizes the entropy, consistent with the constraints.

As we shall see, this principle has some pleasing consequences and some interesting applications to statistical inference. However, carrying out the calculations requires mathematical techniques that are beyond the scope of this book. The problem in general involves maximizing a non-linear, multivariable function over a constraint space. In the comparatively few cases where this can be done exactly, this requires multivariable calculus; in most cases, it requires using techniques of numerical optimization. Therefore we will state these consequences below, and we will describe some applications, but we will only prove one very simple case.

One very helpful feature of the entropy function, in either technique, is that entropy is a *strictly convex* function.[2] If the constraints are likewise convex then (a) there is a unique local maximum, which is the true maximum; (b) basic optimization techniques are guaranteed to converge to the true maximum.

13.6.1 Consequences of the maximum entropy principle

Principle of Indifference: If all you know about X is that it has k different values, then the uniform distribution $P(X = v) = 1/k$ is the maximum entropy distribution. By the maximum entropy principle, you should assume that $P(X = v) = 1/k$. This rule, of course, long predates the principle of maximum entropy; it is known as the *principle of indifference*.

We will prove this in the case $k = 2$; this is the only consequence of the maximum entropy principle that we will actually prove. If p is the probability of one value, then $1 - p$ is the value of the other. Thus, we are looking for the value of p that maximizes $\text{Ent}(p, 1-p) = -(p\log(p)+(1-p)\log(1-p))$. Multiplying this expressing through by $\ln(2)$ it becomes $-(p\ln(p) + (1-p)\ln(1-p))$ which clearly has the same maximum, but is easier to manipulate. Let us call this $f(p)$. The function f attains its maximum when $df/dp = 0$. Thus, $0 = df/dp = -(\ln(p)+1-\ln(1-p)-1)$. So $\ln(p)-\ln(1-p) = 0$; so $\ln(p) = \ln(1-p)$, so $p = 1-p$, so $p = 1/2$.

Independent Events: Suppose that you know the probability distribution on X and the probability distribution on Y. Then the maximum entropy distribution on X, Y is the one for which X and Y are independent.

Specifically: Suppose that you know $P(X = u) = p_u$ and $P(Y = v) = q_v$ for all values of v and u. Let $r_{u,v} = P(X = u, Y = v)$ be the unknown joint probability distribution over X, Y. Then we wish to maximize $\text{Ent}(\{r_{u,v}\})$ subject to the constraints $\sum_v r_{u,v} = p_u$ and $\sum_u r_{u,v} = q_v$. That maximum is attained with $r_{u,v} = p_u \cdot q_v$. (See (Davis 1990 pp. 133-135) for the proof.)

This can also be conditionalized: If $P(E|G)$, $P(F|G)$, $P(E|\neg G)$ and $P(F|\neg G)$ are specified, then the maximum likelihood assumption is that E and F are conditionally independent given G and $\neg G$. This is the assumption used in the analysis of independent evidence, section 8.9.1.

It should be noted, however, that the independence assumption is only a consequence of the maximum entropy principle in this particular state of knowledge; it does not follow in other states of knowledge. Suppose, for example, that X and Y are Boolean random variables, and that you know

[2] A function $f(\vec{v})$ is strictly convex if, for all $\vec{v}, \vec{u}$ and for all t such that $0 < t < 1$, $f(t\vec{v}+(1-t)\vec{u}) > tf(\vec{v})+(1-t)f(\vec{u})$. A constraint $C(\vec{v})$ is convex if if, for all $\vec{v}, \vec{u}$ satisfying C and for all t between 0 and 1, $t\vec{v} + (1-t)\vec{u})$ satisfies C.

$P(X = t) = 1/10$ and that $P(X = t, Y = t) = 1/50$. You might want to conclude, absent other information, that X can be taken to be independent of Y and thus a random sample of Y, and that therefore $P(Y = t) = 1/5$. However, the maximum entropy principle does not at all support you in this. Rather, for the two unknown events, $X = f, Y = t$ and $X = f, Y = f$, it simply divides up the remaining probability evenly, and decides that $P(X = f, Y = t) = P(X = f, Y = f) = 9/20$. Therefore $P(Y = t) = 47/100$.

The problem is that the entropy function over X, Y treats the four events $\langle X = t, Y = t\rangle$; $\langle X = t, Y = f\rangle$; $\langle X = f, Y = t\rangle$; $\langle X = f, Y = f\rangle$ as just four separate, atomic, values $\{tt, tf, ft, ff\}$ of the joint random variable $J = \langle X, Y\rangle$. The function loses track of the fact that these come from X and Y. Once it has done that, it has no reason to suspect that you are particularly interested in the event $Y = t$ which is $J = tt \cup J = ft$. You might just as well be interested in the event $Q = t$, defined as $J = tt \cup J = ff$. The maximum entropy calculation has no less reason to think that Q is independent of X than that Y is independent of X. But both statements cannot be true, and in fact it makes neither assumption.

Uniform distribution: If all you know about the continuous random variable X is that it is 0 outside the interval $[L, U]$, then the maximum entropy density function is the uniform distribution over $[L, U]$.

Normal distribution: If all you know about the continuous random variable X is that $\text{Exp}(X) = \mu$ and $\text{Std}(X) = \sigma$, then the maximum entropy density function is the normal distribution $N_{\mu,\sigma}$.

13.7 Statistical inference

In the maximum entropy approach to statistical inference, you posit constraints that state that the actual probability of certain events is equal to their frequency in the data corpus; and then you maximize the entropy relative to those constraints.

For example, the following entropy-based approach for automated machine translation technique is discussed in (Berger, Della Pietra, and Della Pietra, 1996). You start with a corpus of parallel texts, such as the Canadian Hansard, which is the proceedings of the Canadian Parliament, published in English and French. You want to use the information in this corpus to translate a new text.

Let us suppose, for simplicity, that words in the French can be matched one-to-one with words in the English, and let us further suppose that this matching has been carried out. The problem still remains that the same word in one language is translated into the other in different ways, depending on its meaning, its syntactic function, its context, and so on. For example, the English word "run" is translated in Hansards as "épuiser," "manquer", "écouler", "accumular". "aller", "candidat", "diriger" and others. (The most obvious translation, "courir" meaning the physical activity, does not occur much in Hansards – the subject matter of Parliamentary debate is somewhat specialized.)

As clues to correct translation for word W in sentence S, we will use the three words that precede W in S and the three words that follow W in S. Those six words give a large measure of context which in most cases is sufficient to choose the correct translation. A human reader seeing only the seven word segment of the sentence can generally pick the right translation for the word.[3]

Thus, for each English word e, for each possible translation f for and each set of six context words $c_1, c_2, c_3, c_4, c_5, c_6$, we wish to calculate the probability $P(Tr(e) = f|Context = \langle c_1, c_2, c_3, \cdot c_4, c_5, c_6\rangle)$. For example in translating the word "run" in the sentence, "Harold Albeck plans to run for Comptroller

[3]This has to be modified, of course, for the first three and last three words in the sentence, but the modification is straightforward. Essentially, you view every sentence as being separated from the next by three periods, and you take these periods as "words".

of New York in 2011", we consider

$$P(Tr(\text{“}run''\text{)} = f \mid Context = \langle \text{ “Albeck”, “plans”, “to” } \cdot \text{ ‘for’, “Comptroller” “of” } \rangle),$$

and then we choose the value of f for which this is maximal. Thus, for each English word e we have a probabilistic model of its translation in which the elementary events are tuples of the form $\langle f, c_1 \ldots c_6 \rangle$.

However, of course, this particular sequence of seven words "Albeck plans to run for Comptroller of" almost certainly never occurs in Hansards, so we cannot calculate the above probability directly. Instead, we do the following:

1. Identify a (large) number of patterns that are helpful in disambiguating "run", such as "either c_4, c_5, or c_6 is the word 'for'," or "c_3 is 'to'."
2. Conceptually, characterize each such pattern as the union of elementary events.
3. Impose the constraint that the conditional probability of the translation given the pattern is equal to the conditional frequency of the pattern given the translation.
4. Find the maximum entropy solution for the elementary probabilities subject to the constraints in (3).

The wording of (4) above suggests that one would have to precompute a probability for *every* possible translation of *every* word in *every* possible context of six words. Of course, such a huge distribution could not even be stored, let alone calculated. All we need is the relative conditional probabilities for the context that actually occurs in the sentence being translated; and this can be computed from the relevant patterns. However, the solution is the same as if we had carried out the immense calculation described above.

Exercises

Exercise 13.1

Compute the following quantities (use MATLAB)

A. Ent$(1/3, 1/3, 1/3)$.

B. Ent$(1/4, 1/4, 1/2)$.

C. Ent$(1/5, 2/5, 2/5)$.

D. Ent$(1/10, 1/10, 8/10)$.

Exercise 13.2

Let X be a random variables with values a, b, c, d and let Y be a random variable with values p, q, r with the following joint distribution:

	a	b	c	d
p	0.2	0.05	0.02	0.03
q	0.01	0.04	0.08	0.07
r	0.1	0.3	0.04	0.06

Using MATLAB compute the following quantities: $\mathrm{Ent}(X)$, $\mathrm{Ent}(Y)$, $\mathrm{Ent}(X,Y)$, $\mathrm{Ent}(X|Y=p)$, $\mathrm{CEnt}(X|Y)$, $\mathrm{CEnt}(Y|X)$, $\mathrm{MInf}(X,Y)$.

Exercise 13.3

Given the prefix-free code

$$\text{'a'} \to 00 \quad \text{'b'} \to 01 \quad \text{'c'} \to 100 \quad \text{'d'} \to 101 \quad \text{'e'} \to 110 \quad \text{'f'} \to 111$$

decode the following string: "011011100101110111000111O"

Exercise 13.4

Suppose that $P(\text{'a'})$=0.4; $P(\text{'b'})$=0.15; $P(\text{'c'})$=0.14; $P(\text{'d'})$=0.12; $P(\text{'e'})$=0.1; $P(\text{'f'})$=0.09.

A. What is the entropy of this distribution? (Use MATLAB.)

B. What is the BpC of the code in exercise 13.3 relative to this distribution?

C. Find the Huffman code for this distribution.

D. What is the BpC of the Huffman code for this distribution?

Exercise 13.5

(Use MATLAB.) In section 13.6.1 it is claimed that, given the distributions of two random variables X and Y, the maximum entropy for the joint distribution is achieved when the two variables are independent.

Suppose we have two three-valued random variables X and Y with the distributions

$$\begin{array}{lll} P(X=a)=0.6 & P(X=b)=0.3 & P(X=c)=0.1 \\ P(Y=1)=0.8 & P(Y=2)=0.1 & P(Y=3)=0.1 \end{array}$$

A. Compute the entropy of the joint distribution of X,Y on the assumption that X and Y are independent.

B. Construct a different joint distribution for X,Y which is consistent with these constraints, and compute its entropy.

Problems

Problem 13.1

What is the entropy of the binomial distribution $B_{n,p}(k)$? Hint: If you use theorem 13.1, this is an easy problem. If you start to write down the terms of the binomial distribution, you are entirely on the wrong track.

Chapter 14

Maximum Likelihood Estimation

In this chapter, we discuss maximum likelihood estimation (MLE), one of the basic techniques of classical statistics.

Suppose that you have a collection of data, and that you have some reason to believe that this data was generated by a random process of some specific category, with some unknown parameters. Based on the data, you want to estimate the value of these parameters. For example:

1. The data is the result of randomly sampling k items out of a population of size n and testing each item for a specified property. The actual frequency of the property in the population is an unknown value p. You want to estimate p. This is the sampling problem, discussed in chapter 11, and in section 14.1 below.
2. The data is the result of independent samples of a normal distribution $N_{\mu,\sigma}$ where μ and σ are unknown. You want to estimate the values of μ and σ. This will be discussed in section 14.4 below.

We will also discuss several other similar problems in this chapter.

The problem, then, is to determine the parameters of the process from the data. This can be cast in probabilistic terms as follows: Let D be the data. Let V be a random variable that ranges over the possible values of the parameter, in a given problem. In example (1) above, the domain of V is [0,1], the set of possible values of the parameter p; in example (2) the domain of V is $(-\infty, \infty) \times (0, \infty)$, the set of possible values of $\langle \mu, \sigma \rangle$; in example (3) the domain of V is $[0, 1] \times (-\infty, \infty) \times (0, \infty) \times (-\infty, \infty) \times (0, \infty)$, the set of possible values of $\langle p, \mu_1, \sigma_1, \mu_2, \sigma_2 \rangle$.

We want to estimate the value of V given D. Casting this in probabilistic terms, we want to say something about the distribution of $P(V|D)$. By Bayes' law, for any value v, $P(V = v|D) = P(D|V = v) \cdot P(V = v)/P(D)$,

The denominator $P(D)$ is a fixed normalization constant, and so does not affect the choice of v.

The term $P(V = v)$ is the prior probability distribution for V; that is, the evaluation of the likelihood of parameter values before you see any data. For example, in section 11.3, we discussed using the uniform distribution over $[0, 1]$ for parameter p in the sampling problem of example 1.

In example 2, however, it is much less apparent what would be a reasonable choice for a prior distribution over $\langle \mu, \sigma \rangle$. Since μ ranges over (∞, ∞) and σ ranges over $(0, \infty)$ there does not exist a uniform distribution; and it is not at all clear what alternative prior distribution would be "reasonable".

Lacking any information about $P(V = v)$, therefore, an approach that is often taken is to ignore this term altogether,[1] and simply look for the value of v that maximizes $P(D|V = v)$ (or $\tilde{P}(D|V = v)$, for continuous models.)

In the remainder of this chapter, we discuss the calculation and application of the maximum likelihood estimate for a number of different kinds of random processes.

14.1 Sampling

Let $\vec{D}$ be a sequence of n bits containing m ones and $n - m$ zeros. Suppose that we conjecture that $\vec{D}$ was produced by n flips of a coin of some weight p. This is the situation analyzed at length in chapter 11. If all we need is the maximum likelihood estimate, the analysis is much simpler; the maximum likelihood estimate of p is just m/n, which is what one would expect.

For example suppose that $n = 7, k = 5$. Then the MLE for p is $5/7 = 0.714$, The probability $P(\vec{D}) = p^5(1-p)^2 = 0.0152$. By contrast, if $p = 1/2$ then $P(\vec{D}) = 0.0078$ and if $p = 3/4$ then $P(\vec{D}) = 0.0148$.

Note: Almost all the derivations of MLE estimates in this chapter require calculus, and most require multivariable calculus. The derivations are at the end of each section. Even if you cannot follow the derivation, you should learn the results.

Derivation: The derivation of the MLE in this case is simple. We have $P(\vec{D}) = p^m \cdot (1-p)^{n-m}$. Let us write $f(p) = p^m \cdot (1-p)^{n-m}$. The function $f(p)$ reaches its maximum when
$0 = \frac{df}{dp} = mp^{m-1}(1-p)^{n-m} - (n-m)p^m(1-p)^{n-m-1}$.
Rearranging the terms and dividing through by $p^{m-1}(1-p)^{n-m-1}$ we get $(n-m)p = m(1-p)$ so $p = m/n$.

14.2 Uniform distribution

Let $\vec{D}$ be a sequence of n real numbers. Suppose that we conjecture that $\vec{D}$ is the output of independent samples of a uniform distribution from L to U, where L and U are unknown. Then the MLE is $L = \min(\vec{D})$ and $U = \max(\vec{D})$.

For example, let $\vec{D} = \langle 0.31, 0.41, 0.59, 0.27, 0.18 \rangle$. Then the maximum likelihood estimate is $[0.18, 0.59]$. For that value $\tilde{P}(\vec{D}) = 1/(0.59 - 0.18)^5 = 86.31$. By contrast, if we choose $L = 0, U = 1$, then $\tilde{P}(\vec{D}) = 1$.

Derivation: Let $X^n_{L,U}$ be the process that generates n independent samples of the uniform distribution over $[L, U]$. Then

$$\tilde{P}(X^n_{L,U} = \vec{D}) = \begin{cases} \frac{1}{(U-L)^n} & \text{if } \vec{D}[i] \in [L, U] \text{ for } i = 1 \ldots n \\ 0 & \text{otherwise} \end{cases}$$

This is maximized when $L = \min(\vec{D})$ and $U = \max(\vec{D})$.

[1] This approach is generally considered inconsistent with the likelihood interpretation of probability, which would *require* instead that the data be combined with some prior distribution over V.

14.3 Gaussian distribution: Known variance

Let $\vec{D}$ be a sequence of n real numbers. Suppose that we conjecture that $\vec{D}$ is the output of independent samples of a Gaussian distribution $N_{\mu,\sigma}$ where σ is a fixed value but μ is unknown. The maximum likelihood estimate for μ is that it is the mean of $\vec{D}$, denoted "Exp($\vec{D}$)": $\text{Exp}(\vec{D}) = \sum_{i=1}^{n} \vec{D}[i]/n$.

For example, let $\vec{D} = \langle 0.31, 0.41, 0.59, 0.27, 0.18 \rangle$ as above, and let $\sigma = 1$. Then the maximum likelihood estimate of μ is $\text{Exp}(\vec{D}) = (0.31 + 0.41 + 0.59 + 0.27 + 0.18)/5 = 0.352$. At that value, the probability density is

$$\tilde{P}(X^n_{\mu,\sigma} = D) = \Pi_{i=1}^{n} \frac{\exp(-(\vec{D}[i] - \mu)^2/2\sigma^2)}{\sqrt{2\pi}\sigma} =$$

$$\frac{\exp(-(0.31 - 0.352)^2/2)}{\sqrt{2\pi}} \cdot \ldots \cdot \frac{\exp(-(0.18 - 0.352)^2/2)}{\sqrt{2\pi}} = 0.0096$$

(To save the reader squinting at complicated superscripts in small font, we will write "exp(x)" for e^x. Do not confuse this with Exp, the expected value.)

By contrast, if we choose $\mu = 0.25$, then $\tilde{P}(X^n_{\mu,\sigma} = D) = 0.0094$. If we choose $\mu = 0.59$ then $\tilde{P}(X^n_{\mu,\sigma} = D) = 0.0084$.

Derivation: Let $X^n_{\mu,\sigma}$ be the process that generates n independent samples of the normal distribution. Then

$$\tilde{P}(X^n_{\mu,\sigma} = \vec{D}) = \Pi_{i=1}^{n} \frac{\exp(-(\vec{D}[i] - \mu)^2/2\sigma^2)}{\sqrt{2\pi}\sigma} = \frac{\exp(-\sum_{i=1}^{n}(\vec{D}[i] - \mu)^2/2\sigma^2)}{(\sqrt{2\pi}\sigma)^n}$$

Obviously, for any fixed value of σ, the above expression is a decreasing function of $\sum_{i=1}^{n}(\vec{D}[i] - \mu)^2$. Call this $f(\mu)$. Thus $\tilde{P}(X^n_{\mu,\sigma} = \vec{D})$ reaches its maximum when $f(\mu)$ reaches a minimum. The minimum is attained when the derivative $df/d\mu = 0$. Thus

$0 = df/d\mu = 2\sum_{i=1}^{n}(\vec{D}[i] - \mu) = 2n\mu - 2\sum_{i=1}^{n} \vec{D}[i]$.

So $\mu = \sum_{i=1}^{n} \vec{D}[i]/n = \text{Exp}(\vec{D})$.

All of the remaining MLE computations we discuss in this chapter are based on Gaussian distributions of one kind or another, so they all involve minimizing sums of squares of some kind. Such minimizations are called *least squares* techniques. In fact, one of the major motivations that leads scientists and statisticians to assume Gaussian distributions is precisely that the assumption leads to these elegant least squares problems.

14.4 Gaussian distribution: Unknown variance

As in section 14.3, let $\vec{D}$ be a sequence of n real numbers, and let us conjecture that $\vec{D}$ is the output of independent samples of a normal distribution $N_{\mu,\sigma}$. However, this time let us suppose that both μ and σ are unknown. The maximum likelihood estimate of μ is again $\text{Exp}(\vec{D})$ The maximum likelihood estimate of σ is calculated as follows. We define the *variance* and the *standard deviation* of $\vec{D}$ as $\text{Var}(\vec{D}) = \sum_{i=1}^{n}(\vec{D} - \mu)^2/n$, and $\text{Std}(\vec{D}) = \sqrt{\text{Var}(D)}$. The maximum likelihood estimate of σ is $\text{Std}(\vec{D})$.

The mean, variance, and standard deviation of a *data collection* are closely related to the expected value/variance/standard deviation of a *random variable* discussed in chapter 9, and we use the same symbols in both cases, but the distinction should be kept in mind.

For example, let $\vec{D} = \langle 0.31, 0.41, 0.59, 0.27, 0.18\rangle$ as above. The MLE for μ is 0.352 and the MLE for σ is 0.1401. For these values, $\tilde{P}(X^n_{\mu,\sigma} = \vec{D}) = 15.39$. This may be contrasted with the value obtained in the previous section of $\tilde{P}(X^n_{\mu,\sigma} = \vec{D}) = 0.0096$ for $\mu = 0.352, \sigma = 1$.

It is meaningful also to compare this with the probability 86.31 computed in section 14.2 for this same data set with the uniform distribution over $[0.18, 0.59]$. The significance of the comparison is that if we consider a heterogeneous space of models containing both normal and uniform distributions, then the MLE estimate is the uniform distribution over $[0.18, 0.59]$.

For some other statistical purposes, not discussed in this book,[2] the variance of a data collection is calculated as $\sum_{i=1}^n (\vec{D}[i] - \mu)^2/(n-1)$. In particular, in MATLAB the function calls `std(D)` and `var(D)` use the denominator $n-1$. To get the variance/standard deviation computed with denominator n, you have to use the function calls `std(D,1)` and `var(D,1)`. You have to be careful with this.

Derivation: The derivation of the MLE for μ is the same as in section 14.3. The derivation of σ is a little more work. We again start with the expression

$$\tilde{P}(X^n_{\mu,\sigma} = \vec{D}) = \Pi_{i=1}^n \frac{\exp(-(\vec{D}[i] - \mu)^2/2\sigma^2)}{\sqrt{2\pi}\sigma}$$

Note that if σ is close to 0, the p.d.f. $\tilde{P}(X = \vec{D})$ is very small, because the exponent $-\sum_{i=1}^n (\vec{D}[i] - \mu)^2/2\sigma^2)$ is very large and negative; and if σ is very large, then again $\tilde{P}(X = \vec{D})$ is small because the exponent is about 0, the exponential is therefore about 1, so the overall expression has size proportional to $1/\sigma$. Thus, the maximum is reached at some value in between.

Let $g(\sigma) = \ln(\tilde{P}(X^n_{\mu,\sigma} = \vec{D})) = [\sum_{i=1}^n -(\vec{D}[i] - \mu)^2/2\sigma^2 - \ln(\sigma)] - \ln(\sqrt{2\pi}) =$
$[\sum_{i=1}^n -(\vec{D}_i - \mu)^2/2\sigma^2] - n\ln(\sigma) - \ln(\sqrt{2\pi})$

The maximum is attained when $0 = \partial g/\partial\sigma = [\sum_{i=1}^n (\vec{D}[i] - \mu)^2/\sigma^3] - n/\sigma$, so
$\sigma^2 = \sum_{i=1}^n (\vec{D}[i] - \mu)^2/n = \mathrm{Var}(\vec{D})$, and $\sigma = \mathrm{Std}(\vec{D})$.

Note that in doing this MLE calculation, it is not correct to ignore the normalization factor $1/\sqrt{2\pi}\sigma$, because it changes from one distribution to another. Normalization factors can be ignored in comparing two probabilities or probability densities from the *same* distribution, but not, generally, in comparing probabilities or densities from two *different* distributions.

14.5 Least squares estimates

Let $D = \{\langle x_1, y_1\rangle, \ldots, \langle x_n, y_n\rangle\}$ be a collection of n two-dimensional vectors. Let us conjecture that the y coordinate is a linear function of the x coordinate $f(x) = ax + b$ plus some noise that follows a normal distribution around $f(x)$ with some fixed standard deviation σ. We take the x-coordinates to be given; we are not concerned with how they have been generated. We wish to find the best values of a and b. Let $X^n_{a,b}$ be the associated distribution. Then

$$\tilde{P}(X^n_{a,b} = D) = \Pi_{i=1}^n \frac{\exp(-(y_i - (ax_i + b))^2/2\sigma^2}{\sqrt{2\pi}\sigma} = \frac{\exp(-(\sum_{i=1}^n (y_i - (ax_i + b))^2/2\sigma^2}{(\sqrt{2\pi}\sigma)^n}$$

For fixed σ, the above expression is maximized for the values of a, b where $\sum_{i=1}^n (y_i - (ax_i + b))^2$ is minimized. The line $y = ax + b$ is the *least squares approximation* of the data. This is the line

[2] This alternative calculation gives an *unbiased* estimate.

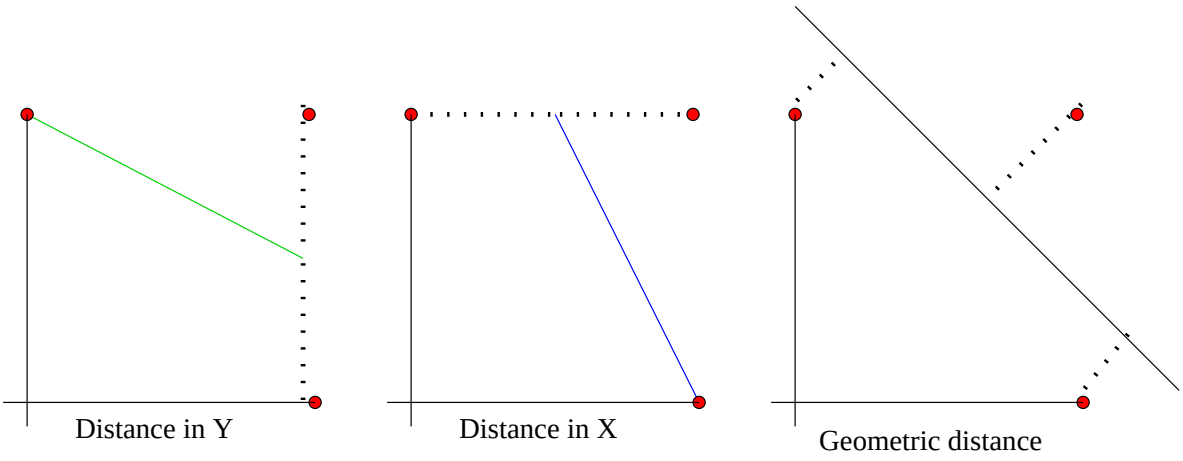


Figure 14.1: Least squares approximations

L that comes "closest" to the points in D, where distance is measured in terms of the sum of the squares of the difference in y-coordinate. That is, you draw a vertical line from each point in D to L, and you compute the sum of the squares of the lengths of the lines. Now find the line L that minimizes that sum.

Note that the line L does *not* minimize the sum of the squares of the geometric distance from the points to the line; that would correspond to normal noise in both the x and y coordinates. We will see in section 14.6 how to solve that problem. Nor does it minimize the sum of the squares of the distance from the points to the line along the x-coordinate, which would correspond to viewing x as a function of y with noise. Each of these three possibilities gives a different line.

For example, consider the data set $D = \{\langle 0,1\rangle, \langle 1,1\rangle, \langle 1,0\rangle\}$. Viewing y as a function of x, the least squares line is $y(x) = 1-0.5x$. The mean square error is $[(1-y(0))^2+(1-y(1)^2+(0-y(1))^2]/3 = 1/6$. Viewing x as a function of y, the least squares line is the $y(x) = 1 - 0.5x$. The mean square error is again $1/6$ (the equality of the two mean square errors is an artifact of the symmetry of the point set, and does not hold in general). The geometrically closest fit is the line $x + y = 4/3$. The mean squared distance from the points to the line is $1/9$ (figure 14.1).

A drawback of the least-squares approximation is that it tends to do badly in the presence of *outliers*: rare erroneous or anomalous cases that lie far away from the general pattern. Since the least squares technique "charges" a cost that is quadratic in the distance, it tends to work hard to try to reduce the distance to the outliers; if the outliers are anomalies or garbage, that is probably misdirected effort. A better estimation function in these cases may be the median approximation, which minimizes the cost function $\sum_i |y_i - (ax_i + b)|$. This corresponds to the maximum likelihood estimate for the random process $Y = aX + b + N$ where the distribution of the noise is given as $P(N = d) = e^{-|d|}/2$. However, the calculation of the MLE for this case is more difficult.

Derivation and formula: Let $f(a,b) = \sum_{i=1}^{n}(y_i - (ax_i + b))^2$. We wish to compute the values of a and b where f is minimal. These can be computed by finding the values of a and b where the partial derivatives of $f(a,b)$ are 0.

$$0 = \frac{\partial f}{\partial a} = \sum_{i=1}^{n} 2x_i \cdot (y_i - (a \cdot x_i + b))$$

$$0 = \frac{\partial f}{\partial b} = \sum_{i=1}^{n} -2(y_i - (a \cdot x_i + b))$$

Collecting common terms in a and b, we get the pair of equations, linear in a and b,

$$\begin{array}{lcll} (\sum_{i=1}^{n} x_i^2)a & + & (\sum_{i=1}^{n} x_i)b & = & \sum_{i=1}^{n} x_i y_i \\ (\sum_{i=1}^{n} x_i a & + & nb & = & \sum_{i=1}^{n} y_i \end{array}$$

For example with the sample set D above, we get the system of equations

$$\begin{array}{lcll} 2a & + & 2b & = & 1 \\ 2a & + & 3b & = & 2 \end{array}$$

The solution is $a = -0.5, b = 1$.

The least squares approximation for a function of an n-dimensional vectors. is similar. Let D be a sequence of pairs $\langle \vec{D}_i, y_i \rangle$, where $\vec{D}$ is a n-dimensional vector. Suppose we conjecture that y is a linear function of $\vec{D}$ plus normal noise; that is $y_i = \vec{a} \bullet \vec{D}_i + b + n_i$ where n_i is normally distributed. We wish to find the maximum likelihood estimate of $\vec{a}$. The analysis is exactly analogous to example 14.5. The MLE estimate for $\vec{a}$ is the value that minimizes $\sum_{i=1}^{n}(y_i - \vec{a} \bullet \vec{D}_i - b)^2$; setting each of the partial derivatives to zeros gives a set of linear equations satisfied by $\vec{a}, b$.

14.5.1 Least squares in MATLAB

As discussed in section 5.4, the MATLAB back-slash operator returns the least-squares solution to an overconstrained system of equations. That is: Let Q be an $m \times n$ matrix such that $\text{Rank}(A) = n < m$ and let $\vec{c}$ be an m-dimensional vector. The system of equations $Q\vec{x} = \vec{c}$ has m equations in n unknowns; in general, it is overconstrained and has no solutions. The MATLAB expression `Q \ c` returns the m-dimensional vector `x` such that $|\vec{c} - Q \cdot \vec{x}|$ is minimal.

We can use this to solve the least-square problem as follows. Let $\{\vec{D}_1 \ldots \vec{D}_m\}$ be a set of m n-dimensional vectors, and let $\vec{Y} = \langle y_1 \ldots y_m \rangle$ be a vector of values. We are looking for the values of $\vec{a}$ and b such that $\sum_i (y_i - (\vec{a} \bullet \vec{D}_i + b))^2$ is minimal. Therefore, construct the $m \times (n+1)$ matrix Q whose ith row is D followed by 1, and call `Q \ Y`. The result is an $n+1$ dimensional vector $\vec{x}$ such that $\vec{x}[1 \ldots n] = \vec{a}$ and $\vec{x}[n+1] = b$.

For example, the least squares calculation in figure 14.1 is carried out as follows:

```
>> Q = [0,1;1,1;1,1];
>> Y = [1;1;0];
>> X=Q\Y;
>> A=X(1)
A =
   -0.5000

>> B=X(2)
B =
    1.0000
```

Another example: Consider the following points

$\vec{D}_1 = \langle 0, 0, 0 \rangle, y_1 = 1;$
$\vec{D}_2 = \langle 0, 1, 1 \rangle, y_2 = 6;$
$\vec{D}_3 = \langle 1, 2, 2 \rangle, y_3 = 12.05;$
$\vec{D}_4 = \langle 2, 1, 0 \rangle, y_4 = 5.03;$
$\vec{D}_5 = \langle 2, 2, 2 \rangle, y_5 = 13.08.$

(These are generated by the function $y = 1+\vec{D}[1]+2\vec{D}[2]+3\vec{D}[3]+0.01\vec{D}[1]^2-0.01\vec{D}[2]^2+0.01\vec{D}[3]^3$.) Then we can find the least squares approximation as follows:

```
>> Q = [0,0,0,1; 0,1,1,1; 1,2,2,1; 2,1,0,1; 2,2,2,1];
>> Y = [1; 6; 12.05; 5.03; 13.08];
>> X=Q\Y;
>> A = X(1:3)
A =
    1.0360
    1.9600
    3.0460

>> B=X(4)
B =
  0.9980
```

As can be seen, the linear part of the function is recovered quite accurately. The accuracy of the approximation can be quantified by computing $\vec{C} = D \cdot \vec{a} + b$ and evaluating $|\vec{C} - \vec{Y}|$

```
>> C= Q(:,1:3)*A +B
C =
    0.9980
    6.0040
   12.0460
    5.0300
   13.0820

>> norm(C-Y)
ans =
    0.0063
```

14.6 Principal component analysis

Principal component analysis is a further variant of the least squares estimate described in sections 14.5. Let $\mathcal{D} = \{\vec{D}_1 \dots \vec{D}_n\}$ be a collection of m-dimensional vectors. We conjecture that the vectors are generated by taking points in some k-dimensional affine space $\mathcal{S}$ and adding a noise vector $\vec{e}$. The direction of the noise $\vec{e}$ is uniformly distributed over the space of vectors orthogonal to $\mathcal{S}$; its length is normally distributed, with variance σ^2. Which subspace $\mathcal{S}$ is the maximum likelihood estimate?

The problem can be solved using the theory of singular value decomposition (SVD) discussed in section 7.7. Let $\vec{\mu}$ be the mean of the vectors in $\mathcal{D}$. Let M be the matrix such that $M[i,:] = \vec{D}_i - \vec{\mu}$. Let $\hat{u}_1 \dots \hat{u}_k$ be the first k right singular vectors of M. Then the space $\{\vec{\mu} + \sum_{i=1}^{k} t_i \hat{u}_i \mid t_i \in \mathbb{R}\}$ is the maximum likelihood estimate.

The right singular vectors $\hat{u}_1 \dots \hat{u}_m$ are called the *principal components* of the data set $\mathcal{D}$, and the process of computing them is *principal component analysis*. Historically, singular value decomposition was developed for use in differential geometry by Beltrami and Jordan, independently, in the 1870's, while principal component analysis was developed for use in statistics by Pearson in 1901.

Another way of viewing principal component analysis is as follows. Define the mean and variance of the collection $\mathcal{D}$ analogously to the mean and variance of a set of numbers: that is, the mean of $\mathcal{D}$ is $\vec{\mu} = \text{Exp}(\mathcal{D}) = \sum_{i=1}^{n} \vec{D}/n$, and the variance of $\mathcal{D}$ is $\text{Var}(\mathcal{D}) = \sum_{i=1}^{n} |\vec{D}_i - \vec{\mu}|^2/n$. (Note that the mean is an m-dimensional vector and the variance is a scalar quantity whose dimension is distance squared.)

The following lemma is easily proven:

Lemma 14.1. *Let D be a collection of m-dimensional vectors. Let $\mathcal{U}$ and $\mathcal{V}$ be orthogonal complements in $\mathbb{R}^m$. Then* $\text{Var}(D) = \text{Var}(\text{Proj}(D,\mathcal{U})) + \text{Var}(\text{Proj}(D,\mathcal{V}))$.

Therefore, the k dimensional subspace $\mathcal{U}$ that maximizes the value of $\text{Var}(\text{Proj}(D,\mathcal{U}))$ is the orthogonal complement of the $m-k$ dimensional subspace $\mathcal{V}$ that minimizes the value of $\text{Var}(\text{Proj}(D,\mathcal{V}))$. We say that the subspace $\mathcal{U}$ *accounts for a fraction f of the variance of D* where $f = \text{Var}(\text{Proj}(D,\mathcal{U})/\text{Var}(D)$. The k dimensional subspace that accounts for the maximal fraction of the variance is thus the subspace spanned by the k first singular vectors; the $m-k$ dimensional subspace that accounts for the minimal fraction of the variance is the subspace spanned by the $m-k$ last singular vectors.

For instance, consider the same data set discussed above: $D = \{\mathbf{a}, \mathbf{b}, \mathbf{c}\}$ where $\mathbf{a} = \langle 1, 0\rangle$, and $\mathbf{b} = \langle 1, 1\rangle$, and $\mathbf{c} = \langle 0, 1\rangle$. The mean of this set is $\mathbf{m} = \langle 2/3, 2/3\rangle$. The total variance $\text{Var}(D) = (d(\mathbf{a},\mathbf{m})^2 + d(\mathbf{b},\mathbf{m})^2 + d(\mathbf{c},\mathbf{m})^2)/3 = (5/9 + 2/9 + 5/9)/3 = 4/9$.

The first principal component is $\hat{u}_1 = \sqrt{2}/2, -\sqrt{2}/2\rangle$ and the second principal component is $\hat{u}_2 = \sqrt{2}/2, +\sqrt{2}/2\rangle$. The principal axes L_1, L_2 are the lines parallel to these through $\mathbf{m} = \langle 2/3, 2/3\rangle$. L_1 is the line $x + y = 4/3$ and L_2 is the line $x = y$. Let $\mathbf{a}_1 = \text{Proj}(\mathbf{a}, L_1) = \langle 1/6, 7/6\rangle$, $\mathbf{b}_1 = \text{Proj}(\mathbf{b}, L_1) = \langle 2/3, 2/3\rangle$, and $\mathbf{c}_1 = \text{Proj}(\mathbf{c}, L_1) = \langle 7/6, 1/6\rangle$. Therefore $\text{Var}(\text{Proj}(D, L_1)) = (d(\mathbf{a}_1,\mathbf{m})^2 + d(\mathbf{b}_1,\mathbf{m})^2 + d(\mathbf{c}_1,\mathbf{m})^2)/3 = (1/2 + 0 + 1/2)/3 = 1/3$.

Likewise, let $\mathbf{a}_2 = \text{Proj}(\mathbf{a}, L_2) = \langle 1/2, 1/2\rangle$, $\mathbf{b}_2 = \text{Proj}(\mathbf{b}, L_2) = \langle 1, 1\rangle$, and $\mathbf{c}_2 = \text{Proj}(\mathbf{c}, L_2) = \langle 1/2, 1/2\rangle$. Therefore $\text{Var}(\text{Proj}(D, L_2)) = (d(\mathbf{a}_2,\mathbf{m})^2 + d(\mathbf{b}_2,\mathbf{m})^2 + d(\mathbf{c}_2,\mathbf{m})^2)/3 = (1/18 + 2/9 + 1/18)/3 = 1/9$.

Thus L_1 accounts for $(1/3)/(4/9) = 3/4$ of the variance and L_2 accounts for $1/4$ of the variance. Note that, as stated in lemma 14.1, $\text{Var}(D) = \text{Var}(\text{Proj}(D), L_1) + \text{Var}(\text{Proj}(D), L_2)$

Derivation: We wish to find the MLE for the following family of models: There exists a k-dimensional affine space $\mathcal{S} \subset R^m$ and n points $\vec{p}_1 \ldots \vec{p}_n$ in $\mathcal{S}$. The data point $\vec{D}_i = \vec{p}_i + q_i\hat{v}_i$ where the distance q_i follows the normal distribution $N_{0,1}$ and $\hat{v}_i$ is uniformly distributed over the space of unit vectors orthogonal to $\mathcal{S}$. The problem is to find the MLE estimate for $\mathcal{S}$ given $\vec{D}_1 \ldots \vec{D}_n$.

There are two parts to the derivation. First, we need to show that the MLE estimate is the one that minimizes the sum of the squares of the distances from the points to the subspace $\mathcal{S}$. This is exactly analogous to the argument for the least squares estimate in section 14.5; we leave the details to the reader.

Second, we need to show that the sum of the squares of the distances is minimized when $\mathcal{S}$ is the affine space through the mean parallel to the first k singular vectors. Let $\vec{p}$ be a point in $\mathcal{S}$. Let $\mathcal{U}$ be the k-dimensional subspace of $\mathbb{R}^m$ parallel to $\mathcal{S}$; that is $\mathcal{U} = \{\vec{s} - \vec{p} | \vec{s} \in \mathcal{S}\}$. Let $\mathcal{V}$ be the orthogonal complement of $\mathcal{U}$, and let $\hat{v}_1 \ldots \hat{v}_{m-k}$ be an orthogonal basis for $\mathcal{V}$.

For any data point $\vec{D}$, $d^2(\vec{D}, \mathcal{S}) = \sum_{j=1}^{m-k}((\vec{D} - \vec{p}) \bullet \hat{v}_j)^2$. Therefore

$$\sum_{i=1}^{n} d^2(\vec{D}_i, \mathcal{S}) = \sum_{i=1}^{n}\sum_{j=1}^{m-k}((\vec{D}_i - \vec{p}) \bullet \hat{v}_j)^2 = \sum_{j=1}^{m-k}\sum_{i=1}^{n}((\vec{D}_i - \vec{p}) \bullet \hat{v}_j)^2$$

For any fixed $\hat{v}_j$ and $\vec{D}_i$, the value of $\sum_{i=1}^{n}((\vec{D}_i - \vec{p}) \bullet \hat{v}_j)^2$ is minimized when the coordinate of $\vec{p}$

in the $\hat{v}_j$ direction is equal to the mean of the coordinates of $\vec{D}_i$ in the $\hat{v}_j$ direction. Therefore, for any fixed choice of $\mathcal{U}$ and $\mathcal{V}$, the minimum is achieved when $\mathcal{S}$ contains the mean $\text{Exp}(D)$.

We can therefore recast the problem as follows: Let $\vec{m} = \text{Exp}(D)$. For $i = 1 \ldots n$, let $\vec{F}_i = \vec{D}_i - \vec{m}$. We wish to find an orthonormal set of vectors $\hat{v}_1 \ldots \hat{v}_{m-k}$ for which $\sum_{i=1}^{n} \sum_{j=1}^{m-k} (\vec{F}_i \cdot \hat{v}_j)^2$ is minimal. Let F be the $n \times m$ matrix whose rows are the $\vec{F}_i$. For any unit vector $\hat{x}$, $F \cdot \hat{x}$ is the column vector $\langle \vec{F}_1 \bullet \hat{x} \ldots \vec{F}_n \bullet \hat{x} \rangle$ so $|F \cdot \hat{x}|^2$ is equal to $(\vec{F}_1 \bullet \hat{x})^2 + \ldots + (\vec{F}_n \bullet \hat{x})^2$. Thus we are looking for a set of orthonormal vectors $\hat{v}_1 \ldots \hat{v}_{m-k}$ that minimizes $\sum_{i=1}^{m-k} |F \bullet \hat{v}_i|^2$. But as we have stated in theorem 7.9, these are the $m - k$ smallest left singular vectors of F.

14.7 Applications of PCA

We will discuss four applications of principal component analysis: for visualization; for data analysis; for finding bounding boxes for graphics and other geometric applications; for finding surface normals; and for clustering related words by their appearance in documents.

14.7.1 PCA for visualization

Suppose that you have a collection of n-dimensional data points that you want to display in a picture that reveals as much as possible of the structure. That is you want to find the best possible two-dimensional mapping of the data. Assuming that the mapping is a projection onto a plane in $\mathbb{R}^n$, then the "best" plane to choose, under the least-squares measure of "bestness", is the plane whose basis is the first two principal components.

14.7.2 PCA for data analysis

Suppose that we have a data collection D of vectors in $\mathbb{R}^n$. We conjecture that the points in D fundamentally lie on an affine space $\mathcal{S}$ within $\mathbb{R}^n$, and that they are slightly perturbed in the dimensions orthogonal to $\mathcal{S}$ by some small noise. The noise may be due, either to small random processes, or to errors in the process of measurement, or even to floating point roundoff in the processing of the points of D. Assume that the signal to noise ratio is large; specifically, that the variance in each of the dimensions within $\mathcal{S}$ is much larger than the variance in any of the noise dimensions. Then $\mathcal{S}$ can be recovered using the following procedure:

- Let $\vec{\mu} = \text{Exp}(D)$.
- Let M be the matrix whose rows are $\vec{d_i} - \vec{\mu}$, where $\vec{d_i} \in D$.
- Let $\langle \sigma_1 \ldots \sigma_m \rangle$ be the singular values of M, and let $\langle \hat{u}_1 \ldots \hat{u}_n \rangle$ be the right singular vectors of M.
- Look for a sudden drop-off in the sequence of singular values; that is, an index q for which σ_{q+1} is much less than σ_q
- Conjecture that $\mathcal{S}$ is the q-dimensional space $\mathcal{S} = \{\vec{\mu} + t_1\hat{u}_1 + \ldots + t_q\hat{u}_q\}$.

Once $\mathcal{S}$ is recovered, it can be used for a variety of purposes:

- **Prediction.** Given $q-1$ coordinates of a vector $\vec{v}$, predict that the remaining coordinates are those that will place it in the space $\mathcal{S}$.

- **Denoising.** If the dimensions orthogonal to $\mathcal{S}$ are indeed noise, then projecting the data onto $\mathcal{S}$ may improve the quality of the data.
- **Data compression.** Approximate each vector $\vec{d_i} \in D$ by its projection in $\mathcal{S}$. This is a generalization of the lossy data compression technique discussed in section 7.9.3.

Another use of the principal components is to posit that the principal components correspond to separate causal factors that combine to generate the data values. The first principal component is the most important determinant of the value; the second is the second most important, and so on. The fact that these principal components are orthogonal guarantees that these causes are independent. In fact, principal component analysis was first invented for this kind of analysis of the results of intelligence tests. This kind of causal inference, however, lies on shaky ground; for an extensive discussion and critique, see *The Mismeasure of Man,* by Stephen Jay Gould.

14.7.3 Bounding box

In 3-dimensional geometric applications, such as graphics, robotics, and computer-aided design, detailed models of 3-dimensional objects are generally given in terms of surface models with thousands or tens of thousands of surface points. A critical operation with these models is to determine whether two objects intersect. The complete algorithm that gives an accurate answer when the objects are close together is very time-consuming for complex models. Since most pairs of objects are nowhere near intersecting, it is important to have a quick way to determine that two objects do not intersect when they are actually not close to intersecting. A standard approach is to compute a *bounding box* for each object: that is, a rectangular box that contains the entire object. If the bounding boxes do not intersect, then the objects certainly do not intersect. It then becomes a problem to choose the direction of the axes of the bounding box. Ideally one would want to choose the axes that give the box of minimal volume; but that is a difficult problem. A good approximation for this is to use the principal components as the axes.

Figure 14.2 shows a collection of points together with the bounding boxes along the $x - y$ axes and along the principal component axes.

14.7.4 Surface normals

Another problem that arises with 3D surface models is to find the normal at a point. This can be done as follows: Given a surface point $\mathbf{q}_0$ on the surface, find a collection of nearby surface points $\mathbf{q}_1 \ldots \mathbf{q}_k$. Compute the PCA of the points $\langle \mathbf{q}_0 \ldots \mathbf{q}_k \rangle$. Since these points all lie close to the tangent plane at $\mathbf{q}_0$, the tangent plane is approximately given by the first two right singular vectors, so the normal is given by the third right singular vector.

14.7.5 Latent semantic analysis

The following technique, called *latent semantic analysis,* is used for automatically grouping together words of related meaning using their co-occurrence in documents.

Suppose we have an online library of documents, and we want to study the occurrence of words in the documents. In section 2.2 we considered the vector model of documents, in which a document was considered a vector in a vector space whose dimensions correspond to words. Here we take the dual approach. Let us consider a high-dimensional vector space, where each dimension corresponds to one document. A word can then be considered as a vector in this space, where the component of

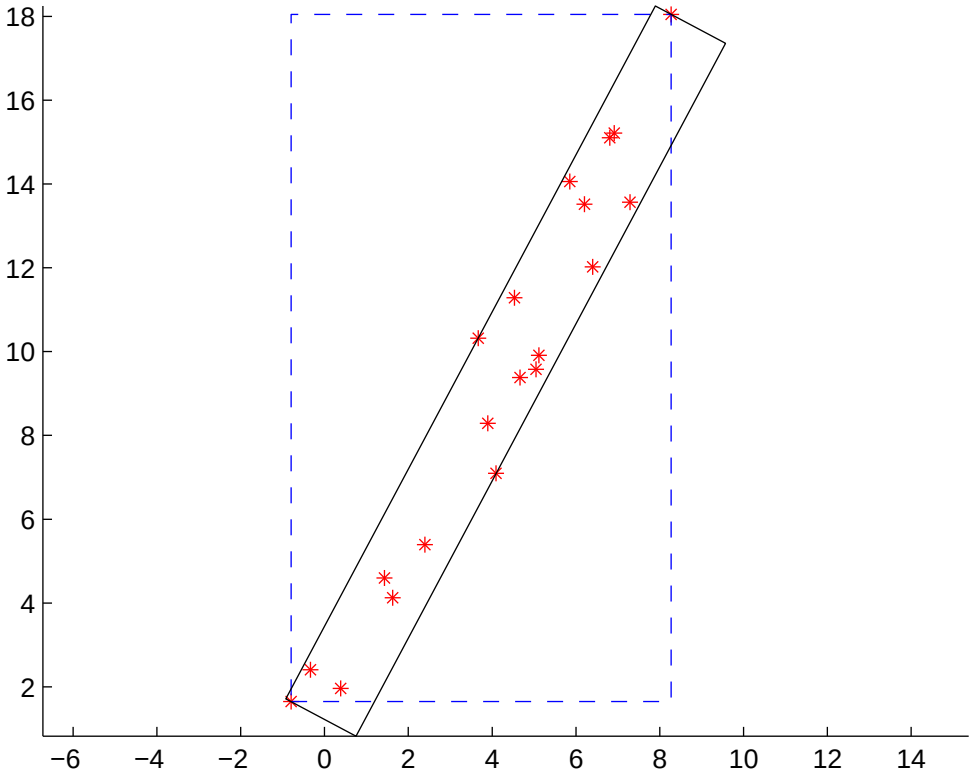


Figure 14.2: Bounding box

word $\vec{w}$ in document d is some measure of the importance of word $\vec{w}$. A cluster of words in document space is thus a collection of words that tend to appear in the same documents and therefore are presumably related. We can find these clusters as follows: (a) normalize all the word vectors to unit length; (b) carry out a PCA of the word vectors; (c) take the top n right singular vectors; (d) for each right singular vector $\hat{u}_i$, form a group G_i of all the words that are nearly parallel to $\hat{u}_i$. (PCA is not an effective way to do clustering in general; it works in this case because the sets of documents corresponding to two different word clusters are substantially disjoint and therefore orthogonal.)

Exercises

All of these exercises require the use of MATLAB.

Exercise 14.1

Suppose that you have sampled 100 items from a large population and found that 75 have a specified property. The formula in 14.1 states that the MLE for the true fraction in the population is $75/100 = 3/4$.

What is the probability of this outcome if the true probability is the MLE 0.75? If the true fraction is 0.7? 0.5? 0.2?

Exercise 14.2

A. Using the MATLAB function `randn`, generate a vector $\vec{D}$ of 10 numbers following the normal distribution $N_{0,1}$. What is the probability density $\tilde{P}(\vec{D})$ of $\vec{D}$ given the distribution $N_{0,1}$?

B. Compute the MLE estimate for the mean μ on the assumption that $\vec{D}$ follows the distribution $N_{\mu,1}$. What is the probability density $\tilde{P}(\vec{D})$ under this distribution?

C. Compute the MLE estimate for the mean μ and standard deviation σ on the assumption that $\vec{D}$ follows the distribution $N_{\mu,\sigma}$. What is the probability density $\tilde{P}(\vec{D})$ under this distribution?

D. Compute the MLE estimate, assuming that $\vec{D}$ was generated by a uniform distribution over the interval $[L, U]$. What is the probability density $\tilde{P}(\vec{D})$ for this estimate?

Exercise 14.3

A. Using the MATLAB function `rand`, generate a vector $\vec{D}$ of 10 numbers following the uniform distribution over [0,1]. What is the probability density $\tilde{P}(D)$ for this distribution?

B-D Repeat exercise 14.2 parts B-D for this new data set.

Exercise 14.4

Consider the following set of 3-dimensional points:

$$\{\ \langle 0,2,1\rangle,\ \langle 0,4,3\rangle,\ \langle 1,4,5\rangle,\ \langle 1,8,6\rangle,\ \langle 1,8,10\rangle,\ \langle 4,8,14\rangle,\ \langle 5,9,13\rangle\ \}$$

A. Find the least squares estimate for z taken as a function of x and y.

B. Find the least squares estimate for x taken as a function of y and z.

C. Find the best-fit plane, in terms of principal component analysis.

Problems

Problem 14.1.

Prove lemma 14.1.

Problem 14.2

Prove that the bounding box for a set of points along the principal component axes is not always equal to the bounding box of minimal volume. Hint: consider what happens to the two rectangles "the bounding box along the principal component axes" and "the bounding box of minimal volume" if you move interior points around.

Programming Assignments

Assignment 14.1

Write a function `InvPowerLawMLE(R,EPS)` which computes the MLE among inverse power laws for a frequency distribution `R`, to accuracy `EPS` > 0. Specifically, `R` is an n-dimensional vector, where `R[I]` is the number of occurrences of the Ith most common element in a sample. Therefore, `R[I]` is a non-increasing function of `I`. Assuming that this sample is generated by an inverse power-law $P(X_I) = \gamma / I^\alpha$ for $I = 1 \ldots N$ where $\alpha > 1$ and γ are constants. Here γ is a normalization factor, whose value depends on α. The function `InvPowerLawMLE(R)` uses numerical binary search to compute the MLE of the parameter α, given a data set `R`.

You should proceed as follows:

- Write a function `InvPowerNormalize(ALPHA,N)` which return the correct normalization factor for given values of α and n.
- Write a function `InvPowerLawProb(ALPHA,F)` which computes the probability of `F` for a given value of α.
- Write the function `InvPowerLawMLE(F)` by doing binary search on values of α. The binary search algorithm for finding a maximum of a continuous function $f(x)$ works as follows: In the first stage, you expand outward from a starting value until you find three values a, b, c such that $f(a) < f(b) > f(c)$. At that point, you can be sure that f has a local maximum between a and c. In the second stage, you work your way inward, testing points either between a and b or between b and c to narrow the range of search for the maximum.

In particular, since the maximum for α is certainly not less than 0, you can execute the following pseudo-code.

```
function m = FindMax(f,eps)
if (f(0) > f(1))
    b = 1/2
    while (f(b) < f(0) && b > eps)
       b = b/2
       end
    c = 2*b
  else
    b = 1
    c = 2
    while (f(b) < f(c))
       b = c;
       c = 2*c;
     end
end
m = BinarySearchForMax(f,eps,a,b,c)
end

function m = BinarySearchForMax(f,eps,a,b,c)
while (c-a > eps)
  if (b-a > c-b)
     d = (a+b)/2
     if (f(d) > f(b))
        c = b
        b = d
      else
        a = d
      end
   else
     d=(b+c)/2
     if (f(d) > f(b))
         a = b
         b = d
      else
         c = d
     end
   end
m = b
end
```

Note: In many applications it would be more reasonable to consider that the distribution holds for $I = 1 \ldots \infty$ rather than $I = 1 \ldots N$. The latter is only valid when you can assume that the sample includes all possible values. However, the computation is more difficult, particularly efficiently computing an accurate value for γ when α is only slightly greater than 1.

Assignment 14.2

In this assignment, you will experiment with latent semantic analysis and dimensionality reduction for data visualization.

Step 1: Choose 5 or 6 related topics; e.g. { math, physics, chemistry, biology, electrical engineering,

astronomy } or { presidents, actors, scientists, writers, composers, athletes }. For each topic, download 20 Wikipedia articles.

Step 2: Do data cleaning: Delete stopwords (see assignment 2.1); delete HTML markup; delete words specific to Wikipedia; delete any word that occurs in only one article.

Step 3: For each remaining word W, the associated *document vector* $\vec{w}$ is the vector whose ith component is the number of occurrences of w in the ith document. Write a program to construct the matrix whose rows are the document vectors for all the remaining words in the corpus.

Step 4: Carry out a principal component analysis of the document vectors.

Step 5: Project the word vectors onto the plane of the first two principal components. Plot the points (or as many of them as you can put in a readable plot) onto an image.

Does the process put closely related words together? Can you attribute any semantic meaning to the two principal components (are these two directions recognizably "about" anything in particular)?

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Mathematical notation

Some notations that are only used in a single section are omitted. The page references here are to the page where the notation is described or defined; therefore standard mathematical notations that are used in the text without explanation have no page reference.

Many of the basic operators are polymorphic; e.g. multiplication can be an operator on two scalars, on a scalar and a vector, etc. This list does not enumerate the different possibilities or provide page references for them.

Special notations

$\vec{v}$ — Vector. 14
$\hat{v}$ — Unit vector.
$\vec{e^i}$ — Unit vector in the ith dimension. 14
$\vec{0}$ — Zero vector. 14
$\vec{1}$ — Vector $\langle 1,1, \ldots 1 \rangle$. 14
$\vec{\Rightarrow}{x}$ — Arrow. 122
$\mathcal{V}$ — Set of vectors.
$\mathbb{R}$ — The real line.
$\mathbb{R}^n$ — Space of n-dimensional vectors.
$\langle x_1 \ldots x_n \rangle$ — n-dimensional vector with components $x_1 \ldots x_n$.
$\{\ldots\}$ — Set.
$e = 2.71828....$ Constant.
$\pi = 3.14159....$ Constant.
$|x|$ — Absolute value of x.
$|\vec{v}|$ — Length of vector $\vec{v}$.
$\begin{bmatrix} a & b & c \\ d & e & f \end{bmatrix}$ Matrix. 40
I_n — $n \times n$ identity matrix. 55
$x \approx y$ — x is approximately equal to y.
$\emptyset$ — Empty set.
$\top$ — True.
$\bot$ — False.
Ω — Sample space.

Operators

$x + y$ — Addition.
$x - y$ — Subtraction.
$x \cdot y$, $x * y$ — Multiplication.
x/y — Division.
$x = y$, $x \neq y$ — Equality, inequality.
$x < y, x > y, x \leq y, x \geq y$ — Order relations.
x^y — Exponentiation.
$\sqrt{x}$ — Square root.
$n!$ — Factorial. 197
$[l, u]$ — Closed interval from l to u.
$\vec{u}[i]$ — ith component of vector $\vec{v}$. 14

$\vec{u} \bullet \vec{v}$ — Dot product. 19.
$M[i, j]$ — Element i, j of matrix M. 40
$M[i, :]$ — ith row of matrix M. 40
$M[:, j]$ — jth column of matrix M. 40
M^{-1} — Matrix inverse. 80
M^T — Matrix transpose. 41
$m \times n$ — m by n (matrix dimension).
$f \circ g$ — Composition of functions f and g. $(f \circ g(x) = f(g(x))$
f^{-1} — Inverse of function f.
$x \in U$ — x is an element of set U.
$U \cup V$ — Set union.
$U \setminus V$ — Set difference.
$U \cap V$ — Set intersection.
$\mathcal{U} \oplus \mathcal{V}$ — Direct sum of vector spaces. 77.
$\neg p$ — Not p.
$p \wedge q$ — p and q.
$p \vee q$ — p or q.
$p \Rightarrow q$ — p implies q.
$p \Leftrightarrow q$ — p if and only if q.
E, F — Joint event of E and F.
X, Y — Joint random variable of X and Y.
$\#_T(E)$ – The number of elements in T satisfying E.
$\sum$ – Summation.
$\prod$ — Product.
$\int$ — Integral.
dx/dt — Derivative.
$\partial x/\partial t$ — Partial derivative.
lim — Limit.
$O(f(n))$ — Order of magnitude growth.

Functions

$B_{n,p}(k)$ — Binomial distribution with parameters n, p. 235
BpC(Γ, X) — Bits per character of coding scheme Γ. X is a probability distribution over an alphabet. 315
C(n, k) — Number of combinations of k out of n. 198.
CEnt$(X|Y)$ — Conditional entropy of random variable X given Y. 313.
Coords$(\vec{v}, \mathcal{B})$ — Coordinates of vector $\vec{v}$ relative to basis $\mathcal{B}$. 73
Coords$(\mathbf{p}, \mathcal{C})$ — Coordinates of point $\mathbf{p}$ relative to coordinate system $\mathcal{C}$. 124.
$\cos(\theta)$ — Trigonometric cosine.
$d(\mathbf{p}, \mathbf{q})$ — Distance between points $\mathbf{p}$ and $\mathbf{q}$. 20
Det(M) — Determinant of matrix M. 137, 147
Dim$(\mathcal{V})$ — Dimension of vector space $\mathcal{V}$. 75
Dir$(\vec{v})$ — Direction of vector $\vec{v}$. 126
Ent(X) — Entropy of random variable X. 311
$\exp(x)$ — Exponent. e^x.
Exp(X) — Expected value of random variable X. 224
Exp(D) — Mean of data set D. 331
Freq$_T(E)$ — Frequency of event E in T.
Hc$(\mathbf{p}, \mathcal{C})$, Hc$(\vec{\vec{x}}, \mathcal{C})$ — Homogeneous coordinates of point $\mathbf{p}$ or arrow $\vec{\vec{x}}$ in coordinate system $\mathcal{C}$. 140

MATLAB notation

The list of Matlab functions and operators includes just those that are mentioned in the text, plus a few additional standard functions. Many of these have many other uses than those mentioned in this index or in the text. The plotting functions are omitted. References are given to the page where the notation is defined or discussed.

MATLAB operators

MATLAB functions

Other MATLAB command and control structures

`while` — While loop. 4

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