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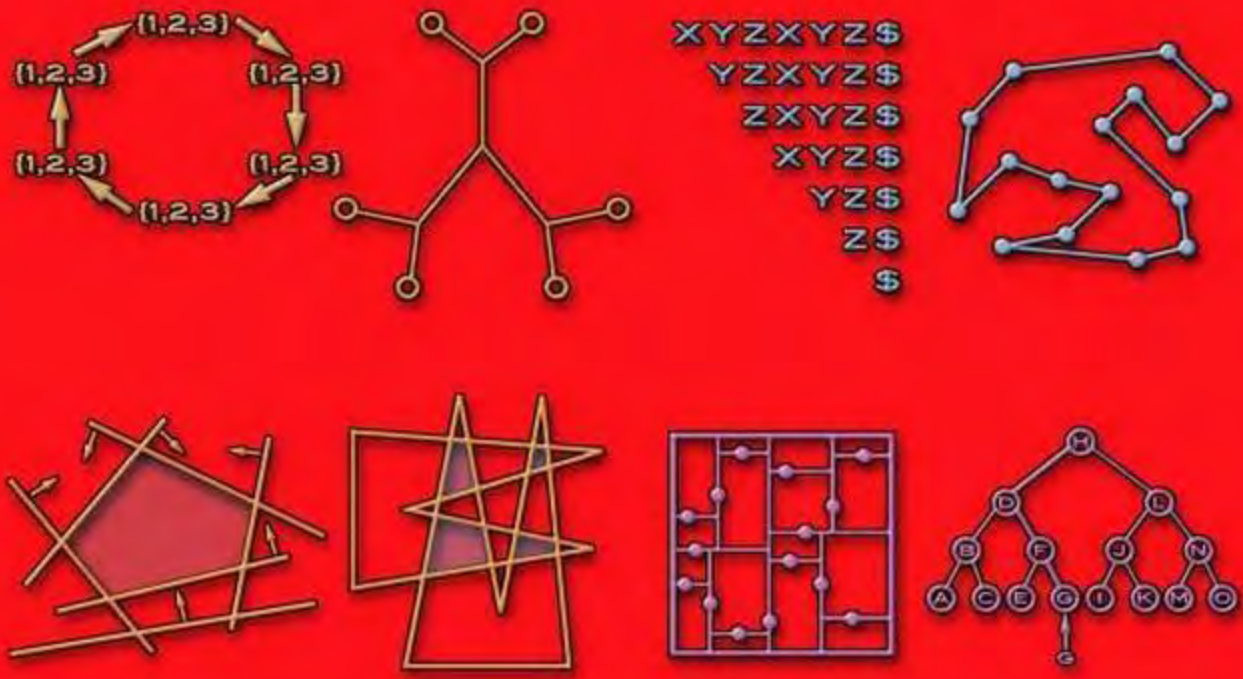
Second Edition

THE Algorithm Design MANUAL



Steven S. Skiena

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Preface

Most professional programmers that I've encountered are not well prepared to tackle algorithm design problems. This is a pity, because the techniques of algorithm design form one of the core practical *technologies* of computer science. Designing correct, efficient, and implementable algorithms for real-world problems requires access to two distinct bodies of knowledge:

- *Techniques* – Good algorithm designers understand several fundamental algorithm design techniques, including data structures, dynamic programming, depth-first search, backtracking, and heuristics. Perhaps the single most important design technique is *modeling*, the art of abstracting a messy real-world application into a clean problem suitable for algorithmic attack.

- *Resources* – Good algorithm designers stand on the shoulders of giants. Rather than laboring from scratch to produce a new algorithm for every task, they can figure out what is known about a particular problem. Rather than re-implementing popular algorithms from scratch, they seek existing implementations to serve as a starting point. They are familiar with many classic algorithmic problems, which provide sufficient source material to model most any application.

This book is intended as a manual on algorithm design, providing access to combinatorial algorithm technology for both students and computer professionals. It is divided into two parts: *Techniques* and *Resources*. The former is a general guide to techniques for the design and analysis of computer algorithms. The Resources section is intended for browsing and reference, and comprises the catalog of algorithmic resources, implementations, and an extensive bibliography.

To the Reader

I have been gratified by the warm reception the first edition of *The Algorithm Design Manual* has received since its initial publication in 1997. It has been recognized as a unique guide to using algorithmic techniques to solve problems that often arise in practice. But much has changed in the world since the *The Algorithm Design Manual* was first published over ten years ago. Indeed, if we date the origins of modern algorithm design and analysis to about 1970, then roughly 30% of modern algorithmic history has happened since the first coming of *The Algorithm Design Manual*.

Three aspects of *The Algorithm Design Manual* have been particularly beloved: (1) the catalog of algorithmic problems, (2) the war stories, and (3) the electronic component of the book. These features have been preserved and strengthened in this edition:

- *The Catalog of Algorithmic Problems* – Since finding out what is known about an algorithmic problem can be a difficult task, I provide a catalog of the 75 most important problems arising in practice. By browsing through this catalog, the student or practitioner can quickly identify what their problem is called, what is known about it, and how they should proceed to solve it. To aid in problem identification, we include a pair of "before" and "after" pictures for each problem, illustrating the required input and output specifications. One perceptive reviewer called my book "The Hitchhiker's Guide to Algorithms" on the strength of this catalog.

  The catalog is *the* most important part of this book. To update the catalog for this edition, I have solicited feedback from the world's leading experts on each associated problem. Particular attention has been paid to updating the discussion of available software implementations for each problem.

- *War Stories* – In practice, algorithm problems do not arise at the beginning of a large project. Rather, they typically arise as subproblems when it becomes clear that the programmer does not know how to proceed or that the current solution is inadequate.

  To provide a better perspective on how algorithm problems arise in the real world, we include a collection of "war stories," or tales from our experience with real problems. The moral of these stories is that algorithm design and analysis is not just theory, but an important tool to be pulled out and used as needed.

  This edition retains all the original war stories (with updates as appropriate) plus additional new war stories covering external sorting, graph algorithms, simulated annealing, and other topics.

- *Electronic Component* – Since the practical person is usually looking for a program more than an algorithm, we provide pointers to solid implementations whenever they are available. We have collected these implementations

at one central website site (*http://www.cs.sunysb.edu/∼algorith*) for easy retrieval. We have been the number one "Algorithm" site on Google pretty much since the initial publication of the book.

Further, we provide recommendations to make it easier to identify the correct code for the job. With these implementations available, the critical issue in algorithm design becomes properly modeling your application, more so than becoming intimate with the details of the actual algorithm. This focus permeates the entire book.

Equally important is what we do not do in this book. We do not stress the mathematical analysis of algorithms, leaving most of the analysis as informal arguments. You will not find a single theorem anywhere in this book. When more details are needed, the reader should study the cited programs or references. The goal of this manual is to get you going in the right direction as quickly as possible.

To the Instructor

This book covers enough material for a standard *Introduction to Algorithms* course. We assume the reader has completed the equivalent of a second programming course, typically titled *Data Structures* or *Computer Science II*.

A full set of lecture slides for teaching this course is available online at *http://www.algorist.com* . Further, I make available online audio and video lectures using these slides to teach a full-semester algorithm course. Let me help teach your course, by the magic of the Internet!

This book stresses design over analysis. It is suitable for both traditional lecture courses and the new "active learning" method, where the professor does not lecture but instead guides student groups to solve real problems. The "war stories" provide an appropriate introduction to the active learning method.

I have made several pedagogical improvements throughout the book. Textbook-oriented features include:

- *More Leisurely Discussion* – The tutorial material in the first part of the book has been *doubled* over the previous edition. The pages have been devoted to more thorough and careful exposition of fundamental material, instead of adding more specialized topics.

- *False Starts* – Algorithms textbooks generally present important algorithms as a fait accompli, obscuring the ideas involved in designing them and the subtle reasons why other approaches fail. The war stories illustrate such development on certain applied problems, but I have expanded such coverage into classical algorithm design material as well.

- *Stop and Think* – Here I illustrate my thought process as I solve a topic-specific homework problem—false starts and all. I have interspersed such

problem blocks throughout the text to increase the problem-solving activity of my readers. Answers appear immediately following each problem.

- *More and Improved Homework Problems* – This edition of *The Algorithm Design Manual* has twice as many homework exercises as the previous one. Exercises that proved confusing or ambiguous have been improved or replaced. Degree of difficulty ratings (from 1 to 10) have been assigned to all problems.

- *Self-Motivating Exam Design* – In my algorithms courses, I promise the students that *all* midterm and final exam questions will be taken directly from homework problems in this book. This provides a "student-motivated exam," so students know exactly how to study to do well on the exam. I have carefully picked the quantity, variety, and difficulty of homework exercises to make this work; ensuring there are neither too few or too many candidate problems.

- *Take-Home Lessons* – Highlighted "take-home" lesson boxes scattered throughout the text emphasize the big-picture concepts to be gained from the chapter.

- *Links to Programming Challenge Problems* – Each chapter's exercises will contain links to 3-5 relevant "Programming Challenge" problems from *http://www.programming-challenges.com*. These can be used to add a programming component to paper-and-pencil algorithms courses.

- *More Code, Less Pseudo-code* – More algorithms in this book appear as code (written in C) instead of pseudo-code. I believe the concreteness and reliability of actual tested implementations provides a big win over less formal presentations for simple algorithms. Full implementations are available for study at *http://www.algorist.com* .

- *Chapter Notes* – Each tutorial chapter concludes with a brief notes section, pointing readers to primary sources and additional references.

Acknowledgments

Updating a book dedication after ten years focuses attention on the effects of time. Since the first edition, Renee has become my wife and then the mother of our two children, Bonnie and Abby. My father has left this world, but Mom and my brothers Len and Rob remain a vital presence in my life. I dedicate this book to my family, new and old, here and departed.

I would like to thank several people for their concrete contributions to this new edition. Andrew Gaun and Betson Thomas helped in many ways, particularly in building the infrastructure for the new *http://www.cs.sunysb.edu/∼algorith*and dealing with a variety of manuscript preparation issues. David Gries offered valuable feedback well beyond the call of duty. Himanshu Gupta and Bin Tang bravely

taught courses using a manuscript version of this edition. Thanks also to my Springer-Verlag editors, Wayne Wheeler and Allan Wylde.

A select group of algorithmic sages reviewed sections of the Hitchhiker's guide, sharing their wisdom and alerting me to new developments. Thanks to:

> Ami Amir, Herve Bronnimann, Bernard Chazelle, Chris Chu, Scott Cotton, Yefim Dinitz, Komei Fukuda, Michael Goodrich, Lenny Heath, Cihat Imamoglu, Tao Jiang, David Karger, Giuseppe Liotta, Albert Mao, Silvano Martello, Catherine McGeoch, Kurt Mehlhorn, Scott A. Mitchell, Naceur Meskini, Gene Myers, Gonzalo Navarro, Stephen North, Joe O'Rourke, Mike Paterson, Theo Pavlidis, Seth Pettie, Michel Pocchiola, Bart Preneel, Tomasz Radzik, Edward Reingold, Frank Ruskey, Peter Sanders, Joao Setubal, Jonathan Shewchuk, Robert Skeel, Jens Stoye, Torsten Suel, Bruce Watson, and Uri Zwick.

Several exercises were originated by colleagues or inspired by other texts. Reconstructing the original sources years later can be challenging, but credits for each problem (to the best of my recollection) appear on the website.

It would be rude not to thank important contributors to the original edition. Ricky Bradley and Dario Vlah built up the substantial infrastructure required for the WWW site in a logical and extensible manner. Zhong Li drew most of the catalog figures using xfig. Richard Crandall, Ron Danielson, Takis Metaxas, Dave Miller, Giri Narasimhan, and Joe Zachary all reviewed preliminary versions of the first edition; their thoughtful feedback helped to shape what you see here.

Much of what I know about algorithms I learned along with my graduate students. Several of them (Yaw-Ling Lin, Sundaram Gopalakrishnan, Ting Chen, Francine Evans, Harald Rau, Ricky Bradley, and Dimitris Margaritis) are the real heroes of the war stories related within. My Stony Brook friends and algorithm colleagues Estie Arkin, Michael Bender, Jie Gao, and Joe Mitchell have always been a pleasure to work and be with. Finally, thanks to Michael Brochstein and the rest of the city contingent for revealing a proper life well beyond Stony Brook.

Caveat

It is traditional for the author to magnanimously accept the blame for whatever deficiencies remain. I don't. Any errors, deficiencies, or problems in this book are somebody else's fault, but I would appreciate knowing about them so as to determine who is to blame.

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April 2008

Contents

1

Introduction to Algorithm Design

What is an algorithm? An algorithm is a procedure to accomplish a specific task. An algorithm is the idea behind any reasonable computer program.

To be interesting, an algorithm must solve a general, well-specified *problem*. An algorithmic problem is specified by describing the complete set of *instances* it must work on and of its output after running on one of these instances. This distinction, between a problem and an instance of a problem, is fundamental. For example, the algorithmic *problem* known as *sorting* is defined as follows:

Problem: Sorting
Input: A sequence of n keys $a_1, \ldots, a_n$.
Output: The permutation (reordering) of the input sequence such that $a'_1 \leq a'_2 \leq \cdots \leq a'_{n-1} \leq a'_n$.

An *instance* of sorting might be an array of names, like {*Mike, Bob, Sally, Jill, Jan*}, or a list of numbers like {*154, 245, 568, 324, 654, 324*}. Determining that you are dealing with a general problem is your first step towards solving it.

An *algorithm* is a procedure that takes any of the possible input instances and transforms it to the desired output. There are many different algorithms for solving the problem of sorting. For example, *insertion sort* is a method for sorting that starts with a single element (thus forming a trivially sorted list) and then incrementally inserts the remaining elements so that the list stays sorted. This algorithm, implemented in C, is described below:

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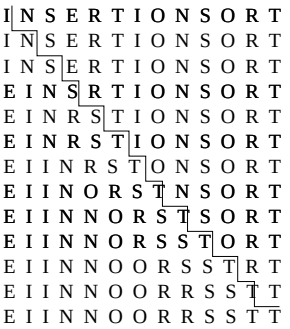

Figure 1.1: Animation of insertion sort in action (time flows down)

```
insertion_sort(item s[], int n)
{
        int i,j;                /* counters */

        for (i=1; i<n; i++) {
                j=i;
                while ((j>0) && (s[j] < s[j-1])) {
                        swap(&s[j],&s[j-1]);
                        j = j-1;
                }
        }
}
```

An animation of the logical flow of this algorithm on a particular instance (the letters in the word "INSERTIONSORT") is given in Figure 1.1

Note the generality of this algorithm. It works just as well on names as it does on numbers, given the appropriate comparison operation ($<$) to test which of the two keys should appear first in sorted order. It can be readily verified that this algorithm correctly orders every possible input instance according to our definition of the sorting problem.

There are three desirable properties for a good algorithm. We seek algorithms that are *correct* and *efficient*, while being *easy to implement*. These goals may not be simultaneously achievable. In industrial settings, any program that seems to give good enough answers without slowing the application down is often acceptable, regardless of whether a better algorithm exists. The issue of finding the best possible answer or achieving maximum efficiency usually arises in industry only after serious performance or legal troubles.

In this chapter, we will focus on the issues of algorithm correctness, and defer a discussion of efficiency concerns to Chapter 2. It is seldom obvious whether a given

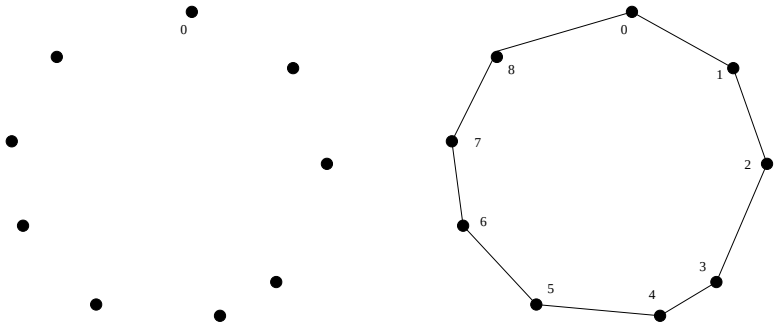

Figure 1.2: A good instance for the nearest-neighbor heuristic

algorithm correctly solves a given problem. Correct algorithms usually come with a proof of correctness, which is an explanation of *why* we know that the algorithm must take every instance of the problem to the desired result. However, before we go further we demonstrate why *"it's obvious"* never suffices as a proof of correctness, and is usually flat-out wrong.

1.1 Robot Tour Optimization

Let's consider a problem that arises often in manufacturing, transportation, and testing applications. Suppose we are given a robot arm equipped with a tool, say a soldering iron. In manufacturing circuit boards, all the chips and other components must be fastened onto the substrate. More specifically, each chip has a set of contact points (or wires) that must be soldered to the board. To program the robot arm for this job, we must first construct an ordering of the contact points so the robot visits (and solders) the first contact point, then the second point, third, and so forth until the job is done. The robot arm then proceeds back to the first contact point to prepare for the next board, thus turning the tool-path into a closed tour, or cycle.

Robots are expensive devices, so we want the tour that minimizes the time it takes to assemble the circuit board. A reasonable assumption is that the robot arm moves with fixed speed, so the time to travel between two points is proportional to their distance. In short, we must solve the following algorithm problem:

Problem: Robot Tour Optimization
Input: A set S of n points in the plane.
Output: What is the shortest cycle tour that visits each point in the set S?

You are given the job of programming the robot arm. Stop right now and think up an algorithm to solve this problem. I'll be happy to wait until you find one...

Several algorithms might come to mind to solve this problem. Perhaps the most popular idea is the *nearest-neighbor* heuristic. Starting from some point p_0, we walk first to its nearest neighbor p_1. From p_1, we walk to its nearest unvisited neighbor, thus excluding only p_0 as a candidate. We now repeat this process until we run out of unvisited points, after which we return to p_0 to close off the tour. Written in pseudo-code, the nearest-neighbor heuristic looks like this:

NearestNeighbor(P)
    Pick and visit an initial point p_0 from P
    $p = p_0$
    $i = 0$
    While there are still unvisited points
        $i = i + 1$
        Select p_i to be the closest unvisited point to p_{i-1}
        Visit p_i
    Return to p_0 from p_{n-1}

This algorithm has a lot to recommend it. It is simple to understand and implement. It makes sense to visit nearby points before we visit faraway points to reduce the total travel time. The algorithm works perfectly on the example in Figure 1.2. The nearest-neighbor rule is reasonably efficient, for it looks at each pair of points (p_i, p_j) at most twice: once when adding p_i to the tour, the other when adding p_j. Against all these positives there is only one problem. This algorithm is completely wrong.

Wrong? How can it be wrong? The algorithm always finds a tour, but it doesn't necessarily find the shortest possible tour. It doesn't necessarily even come close. Consider the set of points in Figure 1.3, all of which lie spaced along a line. The numbers describe the distance that each point lies to the left or right of the point labeled '0'. When we start from the point '0' and repeatedly walk to the nearest unvisited neighbor, we might keep jumping left-right-left-right over '0' as the algorithm offers no advice on how to break ties. A much better (indeed optimal) tour for these points starts from the leftmost point and visits each point as we walk right before returning at the rightmost point.

Try now to imagine your boss's delight as she watches a demo of your robot arm hopscotching left-right-left-right during the assembly of such a simple board.

"But wait," you might be saying. "The problem was in starting at point '0'. Instead, why don't we start the nearest-neighbor rule using the leftmost point as the initial point p_0? By doing this, we will find the optimal solution on this instance."

That is 100% true, at least until we rotate our example 90 degrees. Now all points are equally leftmost. If the point '0' were moved just slightly to the left, it would be picked as the starting point. Now the robot arm will hopscotch up-down-up-down instead of left-right-left-right, but the travel time will be just as bad as before. No matter what you do to pick the first point, the nearest-neighbor rule is doomed to work incorrectly on certain point sets.

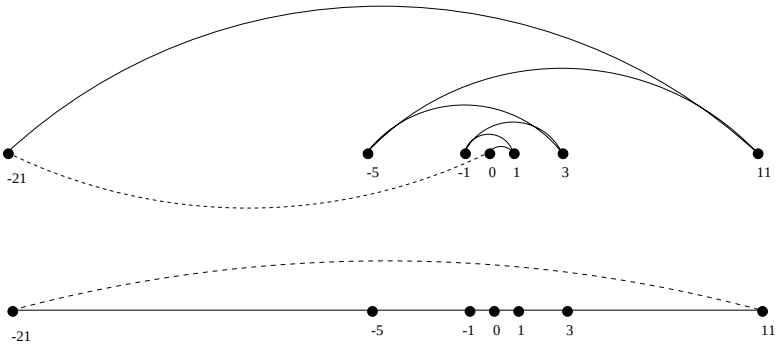

Figure 1.3: A bad instance for the nearest-neighbor heuristic, with the optimal solution

Maybe what we need is a different approach. Always walking to the closest point is too restrictive, since it seems to trap us into making moves we didn't want. A different idea might be to repeatedly connect the closest pair of endpoints whose connection will not create a problem, such as premature termination of the cycle. Each vertex begins as its own single vertex chain. After merging everything together, we will end up with a single chain containing all the points in it. Connecting the final two endpoints gives us a cycle. At any step during the execution of this *closest-pair heuristic*, we will have a set of single vertices and vertex-disjoint chains available to merge. In pseudocode:

ClosestPair(P)
    Let n be the number of points in set P.
    For $i = 1$ to $n - 1$ do
        $d = \infty$
        For each pair of endpoints (s, t) from distinct vertex chains
            if $dist(s, t) \leq d$ then $s_m = s$, $t_m = t$, and $d = dist(s, t)$
        Connect (s_m, t_m) by an edge
    Connect the two endpoints by an edge

This closest-pair rule does the right thing in the example in Figure 1.3. It starts by connecting '0' to its immediate neighbors, the points 1 and -1. Subsequently, the next closest pair will alternate left-right, growing the central path by one link at a time. The closest-pair heuristic is somewhat more complicated and less efficient than the previous one, but at least it gives the right answer in this example.

But this is not true in all examples. Consider what this algorithm does on the point set in Figure 1.4(l). It consists of two rows of equally spaced points, with the rows slightly closer together (distance $1 - e$) than the neighboring points are spaced within each row (distance $1 + e$). Thus the closest pairs of points stretch across the gap, not around the boundary. After we pair off these points, the closest

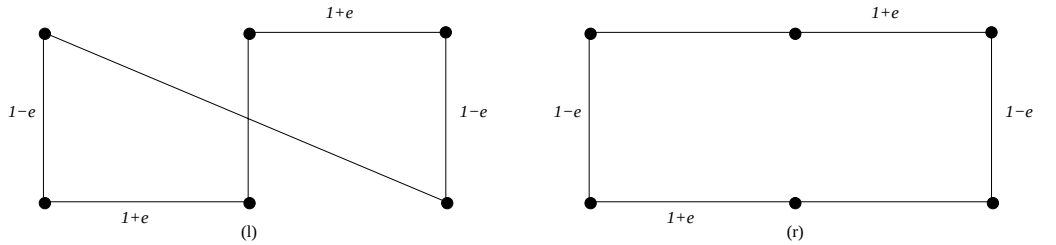

Figure 1.4: A bad instance for the closest-pair heuristic, with the optimal solution

remaining pairs will connect these pairs alternately around the boundary. The total path length of the closest-pair tour is $3(1-e)+2(1+e)+\sqrt{(1-e)^2+(2+2e)^2}$. Compared to the tour shown in Figure 1.4(r), we travel over 20% farther than necessary when $e \approx 0$. Examples exist where the penalty is considerably worse than this.

Thus this second algorithm is also wrong. Which one of these algorithms performs better? You can't tell just by looking at them. Clearly, both heuristics can end up with very bad tours on very innocent-looking input.

At this point, you might wonder what a correct algorithm for our problem looks like. Well, we could try enumerating *all* possible orderings of the set of points, and then select the ordering that minimizes the total length:

```
OptimalTSP(P)
    d = ∞
    For each of the n! permutations P_i of point set P
        If (cost(P_i) ≤ d) then d = cost(P_i) and P_min = P_i
    Return P_min
```

Since all possible orderings are considered, we are guaranteed to end up with the shortest possible tour. This algorithm is correct, since we pick the best of all the possibilities. But it is also extremely slow. The fastest computer in the world couldn't hope to enumerate all the 20! =2,432,902,008,176,640,000 orderings of 20 points within a day. For real circuit boards, where $n \approx 1,000$, forget about it. All of the world's computers working full time wouldn't come close to finishing the problem before the end of the universe, at which point it presumably becomes moot.

The quest for an efficient algorithm to solve this problem, called the *traveling salesman problem* (TSP), will take us through much of this book. If you need to know how the story ends, check out the catalog entry for the traveling salesman problem in Section 16.4 (page 533).

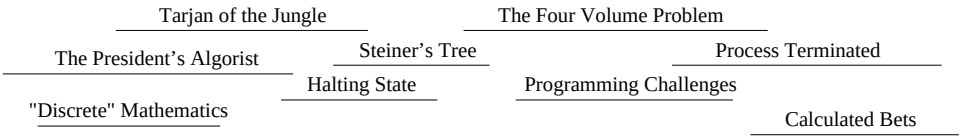

Figure 1.5: An instance of the non-overlapping movie scheduling problem

Take-Home Lesson: There is a fundamental difference between *algorithms*, which always produce a correct result, and *heuristics*, which may usually do a good job but without providing any guarantee.

1.2 Selecting the Right Jobs

Now consider the following scheduling problem. Imagine you are a highly-in-demand actor, who has been presented with offers to star in n different movie projects under development. Each offer comes specified with the first and last day of filming. To take the job, you must commit to being available throughout this entire period. Thus you cannot simultaneously accept two jobs whose intervals overlap.

For an artist such as yourself, the criteria for job acceptance is clear: you want to make as much money as possible. Because each of these films pays the same fee per film, this implies you seek the largest possible set of jobs (intervals) such that no two of them conflict with each other.

For example, consider the available projects in Figure 1.5. We can star in at most four films, namely *"Discrete" Mathematics*, *Programming Challenges*, *Calculated Bets*, and one of either *Halting State* or *Steiner's Tree*.

You (or your agent) must solve the following algorithmic scheduling problem:

Problem: Movie Scheduling Problem
Input: A set I of n intervals on the line.
Output: What is the largest subset of mutually non-overlapping intervals which can be selected from I?

You are given the job of developing a scheduling algorithm for this task. Stop right now and try to find one. Again, I'll be happy to wait.

There are several ideas that may come to mind. One is based on the notion that it is best to work whenever work is available. This implies that you should start with the job with the earliest start date – after all, there is no other job you can work on, then at least during the begining of this period.

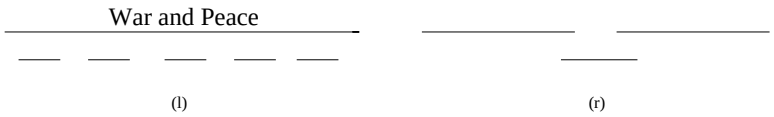

Figure 1.6: Bad instances for the (l) earliest job first and (r) shortest job first heuristics.

EarliestJobFirst(I)
Accept the earlest starting job j from I which does not overlap any previously accepted job, and repeat until no more such jobs remain.

This idea makes sense, at least until we realize that accepting the earliest job might block us from taking many other jobs if that first job is long. Check out Figure 1.6(l), where the epic "War and Peace" is both the first job available and long enough to kill off all other prospects.

This bad example naturally suggests another idea. The problem with "War and Peace" is that it is too long. Perhaps we should start by taking the shortest job, and keep seeking the shortest available job at every turn. Maximizing the number of jobs we do in a given period is clearly connected to banging them out as quickly as possible. This yields the heuristic:

ShortestJobFirst(I)
While ($I \neq \emptyset$) do
Accept the shortest possible job j from I.
Delete j, and any interval which intersects j from I.

Again this idea makes sense, at least until we realize that accepting the shortest job might block us from taking two other jobs, as shown in Figure 1.6(r). While the potential loss here seems smaller than with the previous heuristic, it can readily limit us to half the optimal payoff.

At this point, an algorithm where we try all possibilities may start to look good, because we can be certain it is correct. If we ignore the details of testing whether a set of intervals are in fact disjoint, it looks something like this:

ExhaustiveScheduling(I)
$j = 0$
$S_{max} = \emptyset$
For each of the 2^n subsets S_i of intervals I
If (S_i is mutally non-overlapping) and ($size(S_i) > j$)
then $j = size(S_i)$ and $S_{max} = S_i$.
Return S_{max}

But how slow is it? The key limitation is enumerating the 2^n subsets of n things. The good news is that this is *much* better than enumerating all $n!$ orders

of n things, as proposed for the robot tour optimization problem. There are only about one million subsets when $n = 20$, which could be exhaustively counted within seconds on a decent computer. However, when fed $n = 100$ movies, 2^{100} is much much greater than the 20! which made our robot cry "uncle" in the previous problem.

The difference between our scheduling and robotics problems are that there *is* an algorithm which solves movie scheduling both correctly and efficiently. Think about the first job to terminate—i.e. the interval x which contains the rightmost point which is leftmost among all intervals. This role is played by *"Discrete" Mathematics* in Figure 1.5. Other jobs may well have started before x, but all of these must at least partially overlap each other, so we can select at most one from the group. The first of these jobs to terminate is x, so any of the overlapping jobs potentially block out other opportunities to the right of it. Clearly we can never lose by picking x. This suggests the following correct, efficient algorithm:

```
OptimalScheduling(I)
    While (I ≠ ∅) do
        Accept the job j from I with the earliest completion date.
        Delete j, and any interval which intersects j from I.
```

Ensuring the optimal answer over all possible inputs is a difficult but often achievable goal. Seeking counterexamples that break pretender algorithms is an important part of the algorithm design process. Efficient algorithms are often lurking out there; this book seeks to develop your skills to help you find them.

> *Take-Home Lesson:* Reasonable-looking algorithms can easily be incorrect. Algorithm correctness is a property that must be carefully demonstrated.

1.3 Reasoning about Correctness

Hopefully, the previous examples have opened your eyes to the subtleties of algorithm correctness. We need tools to distinguish correct algorithms from incorrect ones, the primary one of which is called a *proof*.

A proper mathematical proof consists of several parts. First, there is a clear, precise statement of what you are trying to prove. Second, there is a set of assumptions of things which are taken to be true and hence used as part of the proof. Third, there is a chain of reasoning which takes you from these assumptions to the statement you are trying to prove. Finally, there is a little square (∎) or *QED* at the bottom to denote that you have finished, representing the Latin phrase for "thus it is demonstrated."

This book is not going to emphasize formal proofs of correctness, because they are very difficult to do right and quite misleading when you do them wrong. A proof is indeed a *demonstration*. Proofs are useful only when they are honest; crisp arguments explaining why an algorithm satisfies a nontrivial correctness property.

Correct algorithms require careful exposition, and efforts to show both correctness and *not incorrectness*. We develop tools for doing so in the subsections below.

1.3.1 Expressing Algorithms

Reasoning about an algorithm is impossible without a careful description of the sequence of steps to be performed. The three most common forms of algorithmic notation are (1) English, (2) pseudocode, or (3) a real programming language. We will use all three in this book. Pseudocode is perhaps the most mysterious of the bunch, but it is best defined as a programming language that never complains about syntax errors. All three methods are useful because there is a natural tradeoff between greater ease of expression and precision. English is the most natural but least precise programming language, while Java and C/C++ are precise but difficult to write and understand. Pseudocode is generally useful because it represents a happy medium.

The choice of which notation is best depends upon which method you are most comfortable with. I usually prefer to describe the *ideas* of an algorithm in English, moving to a more formal, programming-language-like pseudocode or even real code to clarify sufficiently tricky details.

A common mistake my students make is to use pseudocode to dress up an ill-defined idea so that it looks more formal. Clarity should be the goal. For example, the `ExhaustiveScheduling` algorithm on page 10 could have been better written in English as:

ExhaustiveScheduling(I)
Test all 2^n subsets of intervals from I, and return the largest subset consisting of mutually non-overlapping intervals.

Take-Home Lesson: The heart of any algorithm is an *idea*. If your idea is not clearly revealed when you express an algorithm, then you are using too low-level a notation to describe it.

1.3.2 Problems and Properties

We need more than just an algorithm description in order to demonstrate correctness. We also need a careful description of the problem that it is intended to solve.

Problem specifications have two parts: (1) the set of allowed input instances, and (2) the required properties of the algorithm's output. It is impossible to prove the correctness of an algorithm for a fuzzily-stated problem. Put another way, ask the wrong problem and you will get the wrong answer.

Some problem specifications allow too broad a class of input instances. Suppose we had allowed film projects in our movie scheduling problem to have gaps in

production (i.e. , filming in September and November but a hiatus in October). Then the schedule associated with any particular film would consist of a given *set* of intervals. Our star would be free to take on two interleaving but not overlapping projects (such as the film above nested with one filming in August and October). The earliest completion algorithm would not work for such a generalized scheduling problem. Indeed, *no* efficient algorithm exists for this generalized problem.

> *Take-Home Lesson:* An important and honorable technique in algorithm design is to narrow the set of allowable instances until there *is* a correct and efficient algorithm. For example, we can restrict a graph problem from general graphs down to trees, or a geometric problem from two dimensions down to one.

There are two common traps in specifying the output requirements of a problem. One is asking an ill-defined question. Asking for the *best* route between two places on a map is a silly question unless you define what *best* means. Do you mean the shortest route in total distance, or the fastest route, or the one minimizing the number of turns?

The second trap is creating compound goals. The three path-planning criteria mentioned above are all well-defined goals that lead to correct, efficient optimization algorithms. However, you must pick a single criteria. A goal like *Find the shortest path from a to b that doesn't use more than twice as many turns as necessary* is perfectly well defined, but complicated to reason and solve.

I encourage you to check out the problem statements for each of the 75 catalog problems in the second part of this book. Finding the right formulation for your problem is an important part of solving it. And studying the definition of all these classic algorithm problems will help you recognize when someone else has thought about similar problems before you.

1.3.3 Demonstrating Incorrectness

The best way to prove that an algorithm is *incorrect* is to produce an instance in which it yields an incorrect answer. Such instances are called *counter-examples*. No rational person will ever leap to the defense of an algorithm after a counter-example has been identified. Very simple instances can instantly kill reasonable-looking heuristics with a quick *touché*. Good counter-examples have two important properties:

- *Verifiability* – To demonstrate that a particular instance is a counter-example to a particular algorithm, you must be able to (1) calculate what answer your algorithm will give in this instance, and (2) display a better answer so as to prove the algorithm didn't find it.

  Since you must hold the given instance in your head to reason about it, an important part of verifiability is...

- *Simplicity* – Good counter-examples have all unnecessary details boiled away. They make clear exactly *why* the proposed algorithm fails. Once a counter-example has been found, it is worth simplifying it down to its essence. For example, the counter-example of Figure 1.6(l) could be made simpler and better by reducing the number of overlapped segments from four to two.

Hunting for counter-examples is a skill worth developing. It bears some similarity to the task of developing test sets for computer programs, but relies more on inspiration than exhaustion. Here are some techniques to aid your quest:

- *Think small* – Note that the robot tour counter-examples I presented boiled down to six points or less, and the scheduling counter-examples to only three intervals. This is indicative of the fact that when algorithms fail, there is usually a very simple example on which they fail. Amateur algorists tend to draw a big messy instance and then stare at it helplessly. The pros look carefully at several small examples, because they are easier to verify and reason about.

- *Think exhaustively* – There are only a small number of possibilities for the smallest nontrivial value of n. For example, there are only three interesting ways two intervals on the line can occur: (1) as disjoint intervals, (2) as overlapping intervals, and (3) as properly nesting intervals, one within the other. All cases of three intervals (including counter-examples to both movie heuristics) can be systematically constructed by adding a third segment in each possible way to these three instances.

- *Hunt for the weakness* – If a proposed algorithm is of the form "always take the biggest" (better known as the *greedy algorithm*), think about why that might prove to be the wrong thing to do. In particular, ...

- *Go for a tie* – A devious way to break a greedy heuristic is to provide instances where everything is the same size. Suddenly the heuristic has nothing to base its decision on, and perhaps has the freedom to return something suboptimal as the answer.

- *Seek extremes* – Many counter-examples are mixtures of huge and tiny, left and right, few and many, near and far. It is usually easier to verify or reason about extreme examples than more muddled ones. Consider two tightly bunched clouds of points separated by a much larger distance d. The optimal TSP tour will be essentially $2d$ regardless of the number of points, because what happens within each cloud doesn't really matter.

Take-Home Lesson: Searching for counterexamples is the best way to disprove the correctness of a heuristic.

1.3.4 Induction and Recursion

Failure to find a counterexample to a given algorithm does not mean "it is obvious" that the algorithm is correct. A proof or demonstration of correctness is needed. Often mathematical induction is the method of choice.

When I first learned about mathematical induction it seemed like complete magic. You proved a formula like $\sum_{i=1}^{n} i = n(n+1)/2$ for some basis case like 1 or 2, then *assumed* it was true all the way to $n-1$ before proving it was true for general n using the assumption. That was a proof? Ridiculous!

When I first learned the programming technique of recursion it also seemed like complete magic. The program tested whether the input argument was some basis case like 1 or 2. If not, you solved the bigger case by breaking it into pieces and *calling the subprogram itself* to solve these pieces. That was a program? Ridiculous!

The reason both seemed like magic is because recursion *is* mathematical induction. In both, we have general and boundary conditions, with the general condition breaking the problem into smaller and smaller pieces. The *initial* or boundary condition terminates the recursion. Once you understand either recursion or induction, you should be able to see why the other one also works.

I've heard it said that a computer scientist is a mathematician who only knows how to prove things by induction. This is partially true because computer scientists are lousy at proving things, but primarily because so many of the algorithms we study are either recursive or incremental.

Consider the correctness of *insertion sort*, which we introduced at the beginning of this chapter. The *reason* it is correct can be shown inductively:

- The basis case consists of a single element, and by definition a one-element array is completely sorted.
- In general, we can assume that the first $n-1$ elements of array A are completely sorted after $n-1$ iterations of insertion sort.
- To insert one last element x to A, we find where it goes, namely the unique spot between the biggest element less than or equal to x and the smallest element greater than x. This is done by moving all the greater elements back by one position, creating room for x in the desired location. ∎

One must be suspicious of inductive proofs, however, because very subtle reasoning errors can creep in. The first are *boundary errors*. For example, our insertion sort correctness proof above boldly stated that there was a unique place to insert x between two elements, when our basis case was a single-element array. Greater care is needed to properly deal with the special cases of inserting the minimum or maximum elements.

The second and more common class of inductive proof errors concerns cavallier extension claims. Adding one extra item to a given problem instance might cause the entire optimal solution to change. This was the case in our scheduling problem (see Figure 1.7). The optimal schedule after inserting a new segment may contain

Figure 1.7: Large-scale changes in the optimal solution (boxes) after inserting a single interval (dashed) into the instance

none of the segments of any particular optimal solution prior to insertion. Boldly ignoring such difficulties can lead to very convincing inductive proofs of incorrect algorithms.

Take-Home Lesson: Mathematical induction is usually the right way to verify the correctness of a recursive or incremental insertion algorithm.

Stop and Think: Incremental Correctness

Problem: Prove the correctness of the following recursive algorithm for incrementing natural numbers, i.e. $y \rightarrow y + 1$:

```
Increment(y)
    if y = 0 then return(1) else
        if (y mod 2) = 1 then
            return(2 · Increment(⌊y/2⌋))
        else return(y + 1)
```

Solution: The correctness of this algorithm is certainly *not* obvious to me. But as it is recursive and I am a computer scientist, my natural instinct is to try to prove it by induction.

The basis case of $y = 0$ is obviously correctly handled. Clearly the value 1 is returned, and $0 + 1 = 1$.

Now assume the function works correctly for the general case of $y = n-1$. Given this, we must demonstrate the truth for the case of $y = n$. Half of the cases are easy, namely the even numbers (For which $(y \bmod 2) = 0$), since $y + 1$ is explicitly returned.

For the odd numbers, the answer depends upon what is returned by $Increment(\lfloor y/2 \rfloor)$. Here we want to use our inductive assumption, but it isn't quite right. We have assumed that `increment` worked correctly for $y = n - 1$, but not for a value which is about half of it. We can fix this problem by strengthening our assumption to declare that the general case holds for all $y \leq n-1$. This costs us nothing in principle, but is necessary to establish the correctness of the algorithm.

Now, the case of odd y (i.e. $y = 2m + 1$ for some integer m) can be dealt with as:

$$\begin{aligned} 2 \cdot Increment(\lfloor (2m+1)/2 \rfloor) &= 2 \cdot Increment(\lfloor m + 1/2 \rfloor) \\ &= 2 \cdot Increment(m) \\ &= 2(m+1) \\ &= 2m + 2 = y + 1 \end{aligned}$$

and the general case is resolved. ∎

1.3.5 Summations

Mathematical summation formulae arise often in algorithm analysis, which we will study in Chapter 2. Further, proving the correctness of summation formulae is a classic application of induction. Several exercises on inductive proofs of summations appear as exercises at the end this chapter. To make these more accessible, I review the basics of summations here.

Summation formula are concise expressions describing the addition of an arbitrarily large set of numbers, in particular the formula

$$\sum_{i=1}^{n} f(i) = f(1) + f(2) + \ldots + f(n)$$

There are simple closed forms for summations of many algebraic functions. For example, since n ones is n,

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

The sum of the first n integers can be seen by pairing up the ith and $(n-i+1)$th integers:

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

Recognizing two basic classes of summation formulae will get you a long way in algorithm analysis:

- *Arithmetic progressions* – We already encountered arithmetic progressions when we saw $S(n) = \sum_{i}^{n} i = n(n+1)/2$ in the analysis of selection sort. From the big picture perspective, the important thing is that the sum is quadratic, not that the constant is 1/2. In general,

$$S(n,p) = \sum_{i}^{n} i^p = \Theta(n^{p+1})$$

for $p \geq 1$. Thus the sum of squares is cubic, and the sum of cubes is quartic (if you use such a word). The "big Theta" notation ($\Theta(x)$) will be properly explained in Section 2.2.

For $p < -1$, this sum always converges to a constant, even as $n \to \infty$. The interesting case is between results in ...

- *Geometric series* – In geometric progressions, the index of the loop effects the exponent, i.e.

$$G(n, a) = \sum_{i=0}^{n} a^i = a(a^{n+1} - 1)/(a - 1)$$

How we interpret this sum depends upon the *base* of the progression, i.e. a. When $a < 1$, this converges to a constant even as $n \to \infty$.

This series convergence proves to be the great "free lunch" of algorithm analysis. It means that the sum of a linear number of things can be constant, not linear. For example, $1 + 1/2 + 1/4 + 1/8 + \ldots \leq 2$ no matter how many terms we add up.

When $a > 1$, the sum grows rapidly with each new term, as in $1 + 2 + 4 + 8 + 16 + 32 = 63$. Indeed, $G(n, a) = \Theta(a^{n+1})$ for $a > 1$.

Stop and Think: Factorial Formulae

Problem: Prove that $\sum_{i=1}^{n} i \times i! = (n + 1)! - 1$ by induction.

Solution: The inductive paradigm is straightforward. First verify the basis case (here we do $n = 1$, although $n = 0$ would be even more general):

$$\sum_{i=1}^{1} i \times i! = 1 = (1 + 1)! - 1 = 2 - 1 = 1$$

Now assume the statement is true up to n. To prove the general case of $n + 1$, observe that rolling out the largest term

$$\sum_{i=1}^{n+1} i \times i! = (n + 1) \times (n + 1)! + \sum_{i=1}^{n} i \times i!$$

reveals the left side of our inductive assumption. Substituting the right side gives us

$$\sum_{i=1}^{n+1} i \times i! \quad = \quad (n + 1) \times (n + 1)! + (n + 1)! - 1$$

$$= (n+1)! \times ((n+1)+1) - 1$$
$$= (n+2)! - 1$$

This general trick of separating out the largest term from the summation to reveal an instance of the inductive assumption lies at the heart of all such proofs. ∎

1.4 Modeling the Problem

Modeling is the art of formulating your application in terms of precisely described, well-understood problems. Proper modeling is the key to applying algorithmic design techniques to real-world problems. Indeed, proper modeling can eliminate the need to design or even implement algorithms, by relating your application to what has been done before. Proper modeling is the key to effectively using the "Hitchhiker's Guide" in Part II of this book.

Real-world applications involve real-world objects. You might be working on a system to route traffic in a network, to find the best way to schedule classrooms in a university, or to search for patterns in a corporate database. Most algorithms, however, are designed to work on rigorously defined *abstract* structures such as permutations, graphs, and sets. To exploit the algorithms literature, you must learn to describe your problem abstractly, in terms of procedures on fundamental structures.

1.4.1 Combinatorial Objects

Odds are very good that others have stumbled upon your algorithmic problem before you, perhaps in substantially different contexts. But to find out what is known about your particular "widget optimization problem," you can't hope to look in a book under *widget*. You must formulate widget optimization in terms of computing properties of common structures such as:

- *Permutations* – which are arrangements, or orderings, of items. For example, $\{1, 4, 3, 2\}$ and $\{4, 3, 2, 1\}$ are two distinct permutations of the same set of four integers. We have already seen permutations in the robot optimization problem, and in sorting. Permutations are likely the object in question whenever your problem seeks an "arrangement," "tour," "ordering," or "sequence."

- *Subsets* – which represent selections from a set of items. For example, $\{1, 3, 4\}$ and $\{2\}$ are two distinct subsets of the first four integers. Order does not matter in subsets the way it does with permutations, so the subsets $\{1, 3, 4\}$ and $\{4, 3, 1\}$ would be considered identical. We saw subsets arise in the movie scheduling problem. Subsets are likely the object in question whenever your problem seeks a "cluster," "collection," "committee," "group," "packaging," or "selection."

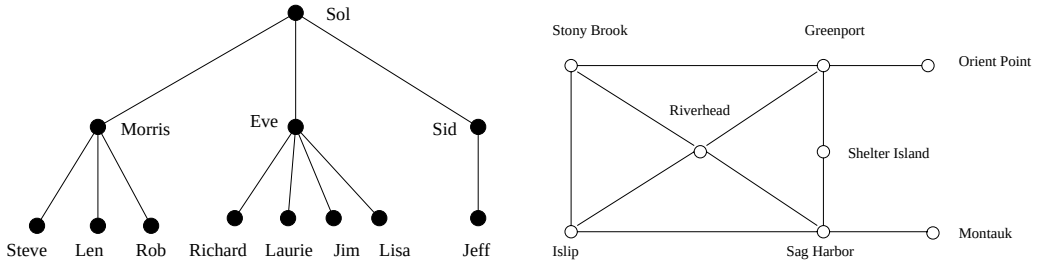

Figure 1.8: Modeling real-world structures with trees and graphs

- *Trees* – which represent hierarchical relationships between items. Figure 1.8(a) shows part of the family tree of the Skiena clan. Trees are likely the object in question whenever your problem seeks a "hierarchy," "dominance relationship," "ancestor/descendant relationship," or "taxonomy."

- *Graphs* – which represent relationships between arbitrary pairs of objects. Figure 1.8(b) models a network of roads as a graph, where the vertices are cities and the edges are roads connecting pairs of cities. Graphs are likely the object in question whenever you seek a "network," "circuit," "web," or "relationship."

- *Points* – which represent locations in some geometric space. For example, the locations of McDonald's restaurants can be described by points on a map/plane. Points are likely the object in question whenever your problems work on "sites," "positions," "data records," or "locations."

- *Polygons* – which represent regions in some geometric spaces. For example, the borders of a country can be described by a polygon on a map/plane. Polygons and polyhedra are likely the object in question whenever you are working on "shapes," "regions," "configurations," or "boundaries."

- *Strings* – which represent sequences of characters or patterns. For example, the names of students in a class can be represented by strings. Strings are likely the object in question whenever you are dealing with "text," "characters," "patterns," or "labels."

These fundamental structures all have associated algorithm problems, which are presented in the catalog of Part II. Familiarity with these problems is important, because they provide the language we use to model applications. To become fluent in this vocabulary, browse through the catalog and study the *input* and *output* pictures for each problem. Understanding these problems, even at a cartoon/definition level, will enable you to know where to look later when the problem arises in your application.

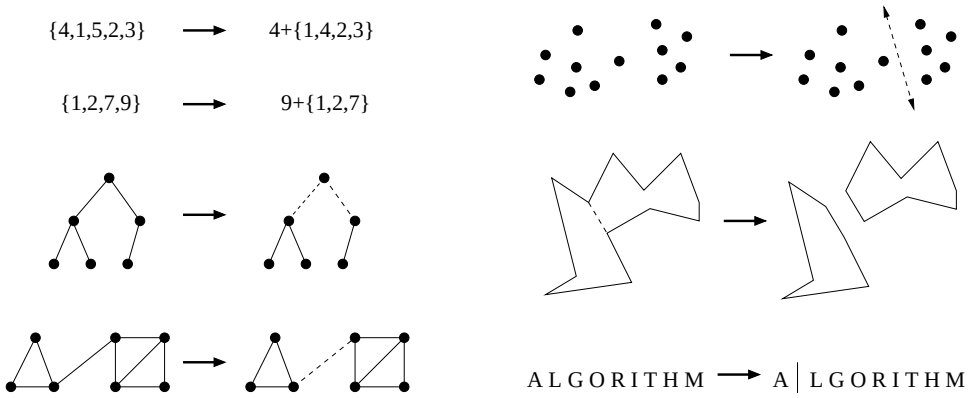

Figure 1.9: Recursive decompositions of combinatorial objects. (left column) Permutations, subsets, trees, and graphs. (right column) Point sets, polygons, and strings

Examples of successful application modeling will be presented in the war stories spaced throughout this book. However, some words of caution are in order. The act of modeling reduces your application to one of a small number of existing problems and structures. Such a process is inherently constraining, and certain details might not fit easily into the given target problem. Also, certain problems can be modeled in several different ways, some much better than others.

Modeling is only the first step in designing an algorithm for a problem. Be alert for how the details of your applications differ from a candidate model, but don't be too quick to say that your problem is unique and special. Temporarily ignoring details that don't fit can free the mind to ask whether they really were fundamental in the first place.

Take-Home Lesson: Modeling your application in terms of well-defined structures and algorithms is the most important single step towards a solution.

1.4.2 Recursive Objects

Learning to think recursively is learning to look for big things that are made from smaller things of *exactly the same type as the big thing*. If you think of houses as sets of rooms, then adding or deleting a room still leaves a house behind.

Recursive structures occur everywhere in the algorithmic world. Indeed, each of the abstract structures described above can be thought about recursively. You just have to see how you can break them down, as shown in Figure 1.9:

- *Permutations* – Delete the first element of a permutation of $\{1, \ldots, n\}$ things and you get a permutation of the remaining $n - 1$ things. Permutations are recursive objects.

- *Subsets* – Every subset of the elements $\{1, \ldots, n\}$ contains a subset of $\{1, \ldots, n-1\}$ made visible by deleting element n if it is present. Subsets are recursive objects.
- *Trees* – Delete the root of a tree and what do you get? A collection of smaller trees. Delete any leaf of a tree and what do you get? A slightly smaller tree. Trees are recursive objects.
- *Graphs* – Delete any vertex from a graph, and you get a smaller graph. Now divide the vertices of a graph into two groups, left and right. Cut through all edges which span from left to right, and what do you get? Two smaller graphs, and a bunch of broken edges. Graphs are recursive objects.
- *Points* – Take a cloud of points, and separate them into two groups by drawing a line. Now you have two smaller clouds of points. Point sets are recursive objects.
- *Polygons* – Inserting any internal chord between two nonadjacent vertices of a simple polygon on n vertices cuts it into two smaller polygons. Polygons are recursive objects.
- *Strings* – Delete the first character from a string, and what do you get? A shorter string. Strings are recursive objects.

Recursive descriptions of objects require both decomposition rules and *basis cases*, namely the specification of the smallest and simplest objects where the decomposition stops. These basis cases are usually easily defined. Permutations and subsets of zero things presumably look like {}. The smallest interesting tree or graph consists of a single vertex, while the smallest interesting point cloud consists of a single point. Polygons are a little trickier; the smallest genuine simple polygon is a triangle. Finally, the empty string has zero characters in it. The decision of whether the basis case contains zero or one element is more a question of taste and convenience than any fundamental principle.

Such recursive decompositions will come to define many of the algorithms we will see in this book. Keep your eyes open for them.

1.5 About the War Stories

The best way to learn how careful algorithm design can have a huge impact on performance is to look at real-world case studies. By carefully studying other people's experiences, we learn how they might apply to our work.

Scattered throughout this text are several of my own algorithmic war stories, presenting our successful (and occasionally unsuccessful) algorithm design efforts on real applications. I hope that you will be able to internalize these experiences so that they will serve as models for your own attacks on problems.

Every one of the war stories is true. Of course, the stories improve somewhat in the retelling, and the dialogue has been punched up to make them more interesting to read. However, I have tried to honestly trace the process of going from a raw problem to a solution, so you can watch how this process unfolded.

The *Oxford English Dictionary* defines an *algorist* as "one skillful in reckonings or figuring." In these stories, I have tried to capture some of the mindset of the algorist in action as they attack a problem.

The various war stories usually involve at least one, and often several, problems from the problem catalog in Part II. I reference the appropriate section of the catalog when such a problem occurs. This emphasizes the benefits of modeling your application in terms of standard algorithm problems. By using the catalog, you will be able to pull out what is known about any given problem whenever it is needed.

1.6 War Story: Psychic Modeling

The call came for me out of the blue as I sat in my office.

"Professor Skiena, I hope you can help me. I'm the President of Lotto Systems Group Inc., and we need an algorithm for a problem arising in our latest product."

"Sure," I replied. After all, the dean of my engineering school is always encouraging our faculty to interact more with industry.

"At Lotto Systems Group, we market a program designed to improve our customers' psychic ability to predict winning lottery numbers.[1] In a standard lottery, each ticket consists of six numbers selected from, say, 1 to 44. Thus, any given ticket has only a very small chance of winning. However, after proper training, our clients can visualize, say, 15 numbers out of the 44 and be certain that at least four of them will be on the winning ticket. Are you with me so far?"

"Probably not," I replied. But then I recalled how my dean encourages us to interact with industry.

"Our problem is this. After the psychic has narrowed the choices down to 15 numbers and is certain that at least 4 of them will be on the winning ticket, we must find the most efficient way to exploit this information. Suppose a cash prize is awarded whenever you pick at least three of the correct numbers on your ticket. We need an algorithm to construct the smallest set of tickets that we must buy in order to guarantee that we win at least one prize."

"Assuming the psychic is correct?"

"Yes, assuming the psychic is correct. We need a program that prints out a list of all the tickets that the psychic should buy in order to minimize their investment. Can you help us?"

Maybe they did have psychic ability, for they had come to the right place. Identifying the best subset of tickets to buy was very much a combinatorial algorithm

[1] Yes, this is a true story.

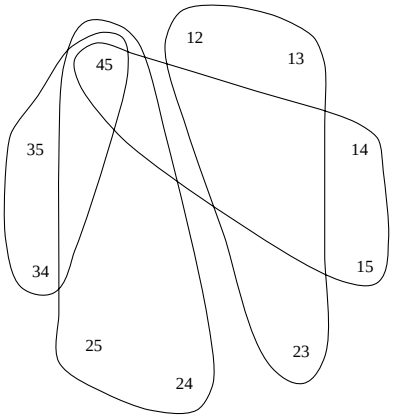

Figure 1.10: Covering all pairs of $\{1, 2, 3, 4, 5\}$ with tickets $\{1, 2, 3\}$, $\{1, 4, 5\}$, $\{2, 4, 5\}$, $\{3, 4, 5\}$

problem. It was going to be some type of covering problem, where each ticket we buy was going to "cover" some of the possible 4-element subsets of the psychic's set. Finding the absolute smallest set of tickets to cover everything was a special instance of the NP-complete problem *set cover* (discussed in Section 18.1 (page 621)), and presumably computationally intractable.

It was indeed a special instance of set cover, completely specified by only four numbers: the size n of the candidate set S (typically $n \approx 15$), the number of slots k for numbers on each ticket (typically $k \approx 6$), the number of psychically-promised correct numbers j from S (say $j = 4$), and finally, the number of matching numbers l necessary to win a prize (say $l = 3$). Figure 1.10 illustrates a covering of a smaller instance, where $n = 5$, $j = k = 3$, and $l = 2$.

"Although it will be hard to find the *exact* minimum set of tickets to buy, with heuristics I should be able to get you pretty close to the cheapest covering ticket set," I told him. "Will that be good enough?"

"So long as it generates better ticket sets than my competitor's program, that will be fine. His system doesn't always guarantee a win. I really appreciate your help on this, Professor Skiena."

"One last thing. If your program can train people to pick lottery winners, why don't you use it to win the lottery yourself?"

"I look forward to talking to you again real soon, Professor Skiena. Thanks for the help."

I hung up the phone and got back to thinking. It seemed like the perfect project to give to a bright undergraduate. After modeling it in terms of sets and subsets, the basic components of a solution seemed fairly straightforward:

- We needed the ability to generate all subsets of k numbers from the candidate set S. Algorithms for generating and ranking/unranking subsets of sets are presented in Section 14.5 (page 452).
- We needed the right formulation of what it meant to have a covering set of purchased tickets. The obvious criteria would be to pick a small set of tickets such that we have purchased at least one ticket containing each of the $\binom{n}{l}$ l-subsets of S that might pay off with the prize.
- We needed to keep track of which prize combinations we have thus far covered. We seek tickets to cover as many thus-far-uncovered prize combinations as possible. The currently covered combinations are a subset of all possible combinations. Data structures for subsets are discussed in Section 12.5 (page 385). The best candidate seemed to be a bit vector, which would answer in constant time "is this combination already covered?"
- We needed a search mechanism to decide which ticket to buy next. For small enough set sizes, we could do an exhaustive search over all possible subsets of tickets and pick the smallest one. For larger problems, a randomized search process like simulated annealing (see Section 7.5.3 (page 254)) would select tickets-to-buy to cover as many uncovered combinations as possible. By repeating this randomized procedure several times and picking the best solution, we would be likely to come up with a good set of tickets.

Excluding the details of the search mechanism, the pseudocode for the bookkeeping looked something like this:

LottoTicketSet(n, k, l)
    Initialize the $\binom{n}{l}$-element bit-vector V to all false
    While there exists a false entry in V
        Select a k-subset T of $\{1, \ldots, n\}$ as the next ticket to buy
        For each of the l-subsets T_i of T, $V[rank(T_i)] = \text{true}$
    Report the set of tickets bought

The bright undergraduate, Fayyaz Younas, rose to the challenge. Based on this framework, he implemented a brute-force search algorithm and found optimal solutions for problems with $n \leq 5$ in a reasonable time. He implemented a random search procedure to solve larger problems, tweaking it for a while before settling on the best variant. Finally, the day arrived when we could call Lotto Systems Group and announce that we had solved the problem.

"Our program found an optimal solution for $n = 15$, $k = 6$, $j = 6$, $l = 3$ meant buying 28 tickets."

"Twenty-eight tickets!" complained the president. "You must have a bug. Look, these five tickets will suffice to cover everything *twice* over: $\{2, 4, 8, 10, 13, 14\}$, $\{4, 5, 7, 8, 12, 15\}$, $\{1, 2, 3, 6, 11, 13\}$, $\{3, 5, 6, 9, 10, 15\}$, $\{1, 7, 9, 11, 12, 14\}$."

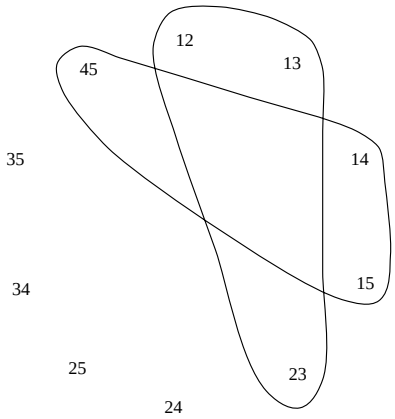

Figure 1.11: Guaranteeing a winning pair from $\{1, 2, 3, 4, 5\}$ using only tickets $\{1, 2, 3\}$ and $\{1, 4, 5\}$

We fiddled with this example for a while before admitting that he was right. *We hadn't modeled the problem correctly!* In fact, we didn't need to explicitly cover all possible winning combinations. Figure 1.11 illustrates the principle by giving a two-ticket solution to our previous four-ticket example. Such unpromising outcomes as $\{2, 3, 4\}$ and $\{3, 4, 5\}$ each agree in one matching pair with tickets from Figure 1.11. We were trying to cover too many combinations, and the penny-pinching psychics were unwilling to pay for such extravagance.

Fortunately, this story has a happy ending. The general outline of our search-based solution still holds for the real problem. All we must fix is which subsets we get credit for covering with a given set of tickets. After this modification, we obtained the kind of results they were hoping for. Lotto Systems Group gratefully accepted our program to incorporate into their product, and hopefully hit the jackpot with it.

The moral of this story is to make sure that you model the problem correctly before trying to solve it. In our case, we came up with a reasonable model, but didn't work hard enough to validate it before we started to program. Our misinterpretation would have become obvious had we worked out a small example by hand and bounced it off our sponsor before beginning work. Our success in recovering from this error is a tribute to the basic correctness of our initial formulation, and our use of well-defined abstractions for such tasks as (1) ranking/unranking k-subsets, (2) the set data structure, and (3) combinatorial search.

Chapter Notes

Every decent algorithm book reflects the design philosophy of its author. For students seeking alternative presentations and viewpoints, we particularly recommend the books of Corman, et. al [CLRS01], Kleinberg/Tardos [KT06], and Manber [Man89].

Formal proofs of algorithm correctness are important, and deserve a fuller discussion than we are able to provide in this chapter. See Gries [Gri89] for a thorough introduction to the techniques of program verification.

The movie scheduling problem represents a very special case of the general *independent set* problem, which is discussed in Section 16.2 (page 528). The restriction limits the allowable input instances to *interval* graphs, where the vertices of the graph G can be represented by intervals on the line and (i, j) is an edge of G iff the intervals overlap. Golumbic [Gol04] provides a full treatment of this interesting and important class of graphs.

Jon Bentley's *Programming Pearls* columns are probably the best known collection of algorithmic "war stories." Originally published in the *Communications of the ACM*, they have been collected in two books [Ben90, Ben99]. Brooks's *The Mythical Man Month* [Bro95] is another wonderful collection of war stories, focused more on software engineering than algorithm design, but they remain a source of considerable wisdom. Every programmer should read all these books, for pleasure as well as insight.

Our solution to the lotto ticket set covering problem is presented in more detail in [YS96].

1.7 Exercises

Finding Counterexamples

1-1. *[3]* Show that $a + b$ can be less than $\min(a, b)$.

1-2. *[3]* Show that $a \times b$ can be less than $\min(a, b)$.

1-3. *[5]* Design/draw a road network with two points a and b such that the fastest route between a and b is not the shortest route.

1-4. *[5]* Design/draw a road network with two points a and b such that the shortest route between a and b is not the route with the fewest turns.

1-5. *[4]* The *knapsack problem* is as follows: given a set of integers $S = \{s_1, s_2, \ldots, s_n\}$, and a target number T, find a subset of S which adds up exactly to T. For example, there exists a subset within $S = \{1, 2, 5, 9, 10\}$ that adds up to $T = 22$ but not $T = 23$.

Find counterexamples to each of the following algorithms for the knapsack problem. That is, giving an S and T such that the subset is selected using the algorithm does not leave the knapsack completely full, even though such a solution exists.

(a) Put the elements of S in the knapsack in left to right order if they fit, i.e. the first-fit algorithm.

(b) Put the elements of S in the knapsack from smallest to largest, i.e. the best-fit algorithm.

(c) Put the elements of S in the knapsack from largest to smallest.

1-6. *[5]* The *set cover problem* is as follows: given a set of subsets $S_1, ..., S_m$ of the universal set $U = \{1, ..., n\}$, find the smallest subset of subsets $T \subset S$ such that $\cup_{t_i \in T} t_i = U$. For example, there are the following subsets, $S_1 = \{1, 3, 5\}$, $S_2 = \{2, 4\}$, $S_3 = \{1, 4\}$, and $S_4 = \{2, 5\}$ The set cover would then be S_1 and S_2.

Find a counterexample for the following algorithm: Select the largest subset for the cover, and then delete all its elements from the universal set. Repeat by adding the subset containing the largest number of uncovered elements until all are covered.

Proofs of Correctness

1-7. *[3]* Prove the correctness of the following recursive algorithm to multiply two natural numbers, for all integer constants $c \geq 2$.

```
function multiply(y, z)
    comment Return the product yz.
1.      if z = 0 then return(0) else
2.      return(multiply(cy, ⌊z/c⌋) + y · (z mod c))
```

1-8. *[3]* Prove the correctness of the following algorithm for evaluating a polynomial. $P(x) = a_n x^n + a_{n-1} x^{n-1} + \ldots + a_1 x + a_0$

```
function horner(A, x)
    p = A_n
    for i from n − 1 to 0
        p = p ∗ x + A_i
    return p
```

1-9. *[3]* Prove the correctness of the following sorting algorithm.

```
function bubblesort (A : list[1 . . . n])
    var int i, j
    for i from n to 1
        for j from 1 to i − 1
            if (A[j] > A[j + 1])
                swap the values of A[j] and A[j + 1]
```

Induction

1-10. *[3]* Prove that $\sum_{i=1}^{n} i = n(n+1)/2$ for $n \geq 0$, by induction.

1-11. *[3]* Prove that $\sum_{i=1}^{n} i^2 = n(n+1)(2n+1)/6$ for $n \geq 0$, by induction.

1-12. *[3]* Prove that $\sum_{i=1}^{n} i^3 = n^2(n+1)^2/4$ for $n \geq 0$, by induction.

1-13. *[3]* Prove that

$$\sum_{i=1}^{n} i(i+1)(i+2) = n(n+1)(n+2)(n+3)/4$$

1-14. *[5]* Prove by induction on $n \geq 1$ that for every $a \neq 1$,

$$\sum_{i=0}^{n} a^i = \frac{a^{n+1} - 1}{a - 1}$$

1-15. *[3]* Prove by induction that for $n \geq 1$,

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

1-16. *[3]* Prove by induction that $n^3 + 2n$ is divisible by 3 for all $n \geq 0$.

1-17. *[3]* Prove by induction that a tree with n vertices has exactly $n - 1$ edges.

1-18. *[3]* Prove by mathematical induction that the sum of the cubes of the first n positive integers is equal to the square of the sum of these integers, i.e.

$$\sum_{i=1}^{n} i^3 = (\sum_{i=1}^{n} i)^2$$

Estimation

1-19. *[3]* Do all the books you own total at least one million pages? How many total pages are stored in your school library?

1-20. *[3]* How many words are there in this textbook?

1-21. *[3]* How many hours are one million seconds? How many days? Answer these questions by doing all arithmetic in your head.

1-22. *[3]* Estimate how many cities and towns there are in the United States.

1-23. *[3]* Estimate how many cubic miles of water flow out of the mouth of the Mississippi River each day. Do not look up any supplemental facts. Describe all assumptions you made in arriving at your answer.

1-24. *[3]* Is disk drive access time normally measured in milliseconds (thousandths of a second) or microseconds (millionths of a second)? Does your RAM memory access a word in more or less than a microsecond? How many instructions can your CPU execute in one year if the machine is left running all the time?

1-25. *[4]* A sorting algorithm takes 1 second to sort 1,000 items on your local machine. How long will it take to sort 10,000 items...

(a) if you believe that the algorithm takes time proportional to n^2, and

(b) if you believe that the algorithm takes time roughly proportional to $n \log n$?

Implementation Projects

1-26. *[5]* Implement the two TSP heuristics of Section 1.1 (page 5). Which of them gives better-quality solutions in practice? Can you devise a heuristic that works better than both of them?

1-27. *[5]* Describe how to test whether a given set of tickets establishes sufficient coverage in the Lotto problem of Section 1.6 (page 23). Write a program to find good ticket sets.

Interview Problems

1-28. *[5]* Write a function to perform integer division without using either the `/` or `*` operators. Find a fast way to do it.

1-29. *[5]* There are 25 horses. At most, 5 horses can race together at a time. You must determine the fastest, second fastest, and third fastest horses. Find the minimum number of races in which this can be done.

1-30. *[3]* How many piano tuners are there in the entire world?

1-31. *[3]* How many gas stations are there in the United States?

1-32. *[3]* How much does the ice in a hockey rink weigh?

1-33. *[3]* How many miles of road are there in the United States?

1-34. *[3]* On average, how many times would you have to flip open the Manhattan phone book at random in order to find a specific name?

Programming Challenges

These programming challenge problems with robot judging are available at *http://www.programming-challenges.com* or *http://online-judge.uva.es*.

1-1. "The $3n + 1$ Problem" – Programming Challenges 110101, UVA Judge 100.

1-2. "The Trip" – Programming Challenges 110103, UVA Judge 10137.

1-3. "Australian Voting" – Programming Challenges 110108, UVA Judge 10142.

2

Algorithm Analysis

Algorithms are the most important and durable part of computer science because they can be studied in a language- and machine-independent way. This means that we need techniques that enable us to compare the efficiency of algorithms without implementing them. Our two most important tools are (1) the RAM model of computation and (2) the asymptotic analysis of worst-case complexity.

Assessing algorithmic performance makes use of the "big Oh" notation that, proves essential to compare algorithms and design more efficient ones. While the hopelessly *practical* person may blanch at the notion of theoretical analysis, we present the material because it really is useful in thinking about algorithms.

This method of keeping score will be the most mathematically demanding part of this book. But once you understand the intuition behind these ideas, the formalism becomes a lot easier to deal with.

2.1 The RAM Model of Computation

Machine-independent algorithm design depends upon a hypothetical computer called the *Random Access Machine* or RAM. Under this model of computation, we are confronted with a computer where:

- Each *simple* operation (+, *, –, =, if, call) takes exactly one time step.
- Loops and subroutines are *not* considered simple operations. Instead, they are the composition of many single-step operations. It makes no sense for *sort* to be a single-step operation, since sorting 1,000,000 items will certainly take much longer than sorting 10 items. The time it takes to run through a loop or execute a subprogram depends upon the number of loop iterations or the specific nature of the subprogram.

S.S. Skiena, *The Algorithm Design Manual*, 2nd ed., DOI: 10.1007/978-1-84800-070-4_2,
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- Each memory access takes exactly one time step. Further, we have as much memory as we need. The RAM model takes no notice of whether an item is in cache or on the disk.

Under the RAM model, we measure run time by counting up the number of steps an algorithm takes on a given problem instance. If we assume that our RAM executes a given number of steps per second, this operation count converts naturally to the actual running time.

The RAM is a simple model of how computers perform. Perhaps it sounds too simple. After all, multiplying two numbers takes more time than adding two numbers on most processors, which violates the first assumption of the model. Fancy compiler loop unrolling and hyperthreading may well violate the second assumption. And certainly memory access times differ greatly depending on whether data sits in cache or on the disk. This makes us zero for three on the truth of our basic assumptions.

And yet, despite these complaints, the RAM proves an *excellent* model for understanding how an algorithm will perform on a real computer. It strikes a fine balance by capturing the essential behavior of computers while being simple to work with. We use the RAM model because it is useful in practice.

Every model has a size range over which it is useful. Take, for example, the model that the Earth is flat. You might argue that this is a bad model, since it has been fairly well established that the Earth is in fact round. But, when laying the foundation of a house, the flat Earth model is sufficiently accurate that it can be reliably used. It is so much easier to manipulate a flat-Earth model that it is inconceivable that you would try to think spherically when you don't have to.[1]

The same situation is true with the RAM model of computation. We make an abstraction that is generally very useful. It is quite difficult to design an algorithm such that the RAM model gives you substantially misleading results. The robustness of the RAM enables us to analyze algorithms in a machine-independent way.

Take-Home Lesson: Algorithms can be understood and studied in a language- and machine-independent manner.

2.1.1 Best, Worst, and Average-Case Complexity

Using the RAM model of computation, we can count how many steps our algorithm takes on any given input instance by executing it. However, to understand how good or bad an algorithm is in general, we must know how it works over *all* instances.

To understand the notions of the best, worst, and average-case complexity, think about running an algorithm over all possible instances of data that can be

[1] The Earth is not completely spherical either, but a spherical Earth provides a useful model for such things as longitude and latitude.

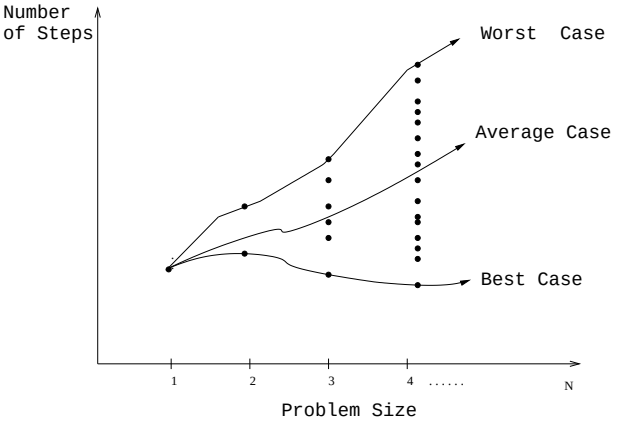

Figure 2.1: Best, worst, and average-case complexity

fed to it. For the problem of sorting, the set of possible input instances consists of all possible arrangements of n keys, over all possible values of n. We can represent each input instance as a point on a graph (shown in Figure 2.1) where the x-axis represents the size of the input problem (for sorting, the number of items to sort), and the y-axis denotes the number of steps taken by the algorithm in this instance.

These points naturally align themselves into columns, because only integers represent possible input size (e.g., it makes no sense to sort 10.57 items). We can define three interesting functions over the plot of these points:

- The *worst-case complexity* of the algorithm is the function defined by the maximum number of steps taken in any instance of size n. This represents the curve passing through the highest point in each column.
- The *best-case complexity* of the algorithm is the function defined by the minimum number of steps taken in any instance of size n. This represents the curve passing through the lowest point of each column.
- The *average-case complexity* of the algorithm, which is the function defined by the average number of steps over all instances of size n.

The worst-case complexity proves to be most useful of these three measures in practice. Many people find this counterintuitive. To illustrate why, try to project what will happen if you bring n dollars into a casino to gamble. The best case, that you walk out owning the place, is possible but so unlikely that you should not even think about it. The worst case, that you lose all n dollars, is easy to calculate and distressingly likely to happen. The average case, that the typical bettor loses 87.32% of the money that he brings to the casino, is difficult to establish and its meaning subject to debate. What exactly does *average* mean? Stupid people lose

more than smart people, so are you smarter or stupider than the average person, and by how much? Card counters at blackjack do better on average than customers who accept three or more free drinks. We avoid all these complexities and obtain a very useful result by just considering the worst case.

The important thing to realize is that each of these time complexities define a numerical function, representing time versus problem size. These functions are as well defined as any other numerical function, be it $y = x^2 - 2x + 1$ or the price of Google stock as a function of time. But time complexities are such complicated functions that we must simplify them to work with them. For this, we need the "Big Oh" notation.

2.2 The Big Oh Notation

The best, worst, and average-case time complexities for any given algorithm are numerical functions over the size of possible problem instances. However, it is very difficult to work precisely with these functions, because they tend to:

- *Have too many bumps* – An algorithm such as binary search typically runs a bit faster for arrays of size exactly $n = 2^k - 1$ (where k is an integer), because the array partitions work out nicely. This detail is not particularly significant, but it warns us that the *exact* time complexity function for any algorithm is liable to be very complicated, with little up and down bumps as shown in Figure 2.2.

- *Require too much detail to specify precisely* – Counting the exact number of RAM instructions executed in the worst case requires the algorithm be specified to the detail of a complete computer program. Further, the precise answer depends upon uninteresting coding details (e.g., did he use a case statement or nested ifs?). Performing a precise worst-case analysis like

  $$T(n) = 12754n^2 + 4353n + 834 \lg_2 n + 13546$$

  would clearly be very difficult work, but provides us little extra information than the observation that "the time grows quadratically with n."

It proves to be much easier to talk in terms of simple upper and lower bounds of time-complexity functions using the Big Oh notation. The Big Oh simplifies our analysis by ignoring levels of detail that do not impact our comparison of algorithms.

The Big Oh notation ignores the difference between multiplicative constants. The functions $f(n) = 2n$ and $g(n) = n$ are identical in Big Oh analysis. This makes sense given our application. Suppose a given algorithm in (say) C language ran twice as fast as one with the same algorithm written in Java. This multiplicative

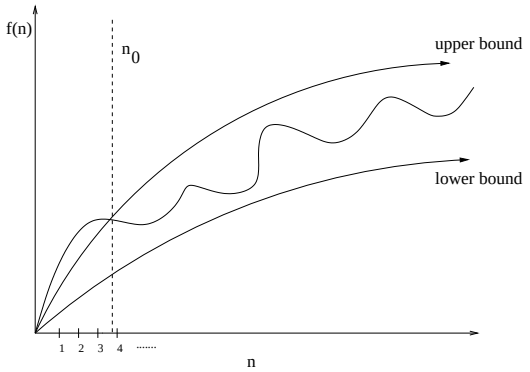

Figure 2.2: Upper and lower bounds valid for $n > n_0$ smooth out the behavior of complex functions

factor of two tells us nothing about the algorithm itself, since both programs implement exactly the same algorithm. We ignore such constant factors when comparing two algorithms.

The formal definitions associated with the Big Oh notation are as follows:

- $f(n) = O(g(n))$ means $c \cdot g(n)$ is an *upper bound* on $f(n)$. Thus there exists some constant c such that $f(n)$ is always $\leq c \cdot g(n)$, for large enough n (i.e. , $n \geq n_0$ for some constant n_0).
- $f(n) = \Omega(g(n))$ means $c \cdot g(n)$ is a *lower bound* on $f(n)$. Thus there exists some constant c such that $f(n)$ is always $\geq c \cdot g(n)$, for all $n \geq n_0$.
- $f(n) = \Theta(g(n))$ means $c_1 \cdot g(n)$ is an upper bound on $f(n)$ and $c_2 \cdot g(n)$ is a lower bound on $f(n)$, for all $n \geq n_0$. Thus there exist constants c_1 and c_2 such that $f(n) \leq c_1 \cdot g(n)$ and $f(n) \geq c_2 \cdot g(n)$. This means that $g(n)$ provides a nice, tight bound on $f(n)$.

Got it? These definitions are illustrated in Figure 2.3. Each of these definitions assumes a constant n_0 beyond which they are always satisfied. We are not concerned about small values of n (i.e. , anything to the left of n_0). After all, we don't really care whether one sorting algorithm sorts six items faster than another, but seek which algorithm proves faster when sorting 10,000 or 1,000,000 items. The Big Oh notation enables us to ignore details and focus on the big picture.

Take-Home Lesson: The Big Oh notation and worst-case analysis are tools that greatly simplify our ability to compare the efficiency of algorithms.

Make sure you understand this notation by working through the following examples. We choose certain constants (c and n_0) in the explanations below because

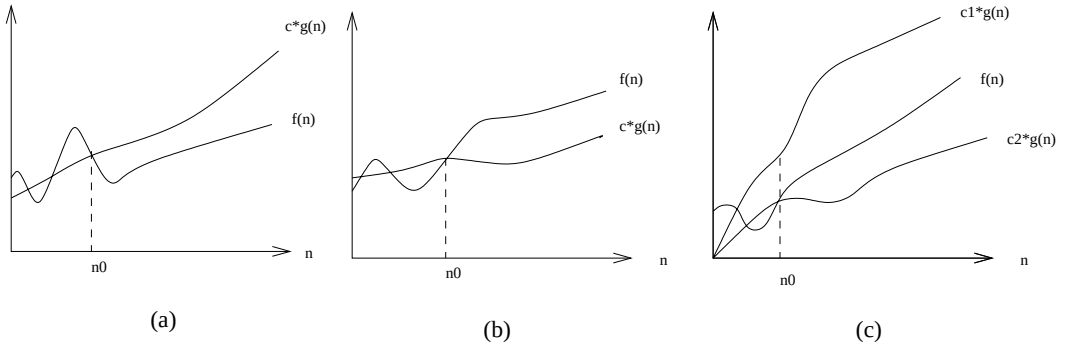

Figure 2.3: Illustrating the big (a) O, (b) Ω, and (c) Θ notations

they work and make a point, but other pairs of constants will do exactly the same job. You are free to choose any constants that maintain the same inequality—ideally constants that make it obvious that the inequality holds:

$3n^2 - 100n + 6 = O(n^2)$, because I choose $c = 3$ and $3n^2 > 3n^2 - 100n + 6$;

$3n^2 - 100n + 6 = O(n^3)$, because I choose $c = 1$ and $n^3 > 3n^2 - 100n + 6$ when $n > 3$;

$3n^2 - 100n + 6 \neq O(n)$, because for any c I choose $c \times n < 3n^2$ when $n > c$;

$3n^2 - 100n + 6 = \Omega(n^2)$, because I choose $c = 2$ and $2n^2 < 3n^2 - 100n + 6$ when $n > 100$;

$3n^2 - 100n + 6 \neq \Omega(n^3)$, because I choose $c = 3$ and $3n^2 - 100n + 6 < n^3$ when $n > 3$;

$3n^2 - 100n + 6 = \Omega(n)$, because for any c I choose $cn < 3n^2 - 100n + 6$ when $n > 100c$;

$3n^2 - 100n + 6 = \Theta(n^2)$, because both O and Ω apply;

$3n^2 - 100n + 6 \neq \Theta(n^3)$, because only O applies;

$3n^2 - 100n + 6 \neq \Theta(n)$, because only Ω applies.

The Big Oh notation provides for a rough notion of equality when comparing functions. It is somewhat jarring to see an expression like $n^2 = O(n^3)$, but its meaning can always be resolved by going back to the definitions in terms of upper and lower bounds. It is perhaps most instructive to read the "=" here as meaning *one of the functions that are*. Clearly, n^2 is one of functions that are $O(n^3)$.

Stop and Think: Back to the Definition

Problem: Is $2^{n+1} = \Theta(2^n)$?

Solution: Designing novel algorithms requires cleverness and inspiration. However, applying the Big Oh notation is best done by swallowing any creative instincts you may have. All Big Oh problems can be correctly solved by going back to the definition and working with that.

- *Is* $2^{n+1} = O(2^n)$*?* Well, $f(n) = O(g(n))$ iff (*if and only if*) there exists a constant c such that for all sufficiently large n $f(n) \leq c \cdot g(n)$. Is there? The key observation is that $2^{n+1} = 2 \cdot 2^n$, so $2 \cdot 2^n \leq c \cdot 2^n$ for any $c \geq 2$.
- *Is* $2^{n+1} = \Omega(2^n)$*?* Go back to the definition. $f(n) = \Omega(g(n))$ iff there exists a constant $c > 0$ such that for all sufficiently large n $f(n) \geq c \cdot g(n)$. This would be satisfied for any $0 < c \leq 2$. Together the Big Oh and Ω bounds imply $2^{n+1} = \Theta(2^n)$

∎

Stop and Think: Hip to the Squares?

Problem: Is $(x + y)^2 = O(x^2 + y^2)$.

Solution: Working with the Big Oh means going back to the definition at the slightest sign of confusion. By definition, this expression is valid iff we can find some c such that $(x + y)^2 \leq c(x^2 + y^2)$.

My first move would be to expand the left side of the equation, i.e. $(x + y)^2 = x^2 + 2xy + y^2$. If the middle $2xy$ term wasn't there, the inequality would clearly hold for any $c > 1$. But it is there, so we need to relate the $2xy$ to $x^2 + y^2$. What if $x \leq y$? Then $2xy \leq 2y^2 \leq 2(x^2 + y^2)$. What if $x \geq y$? Then $2xy \leq 2x^2 \leq 2(x^2 + y^2)$. Either way, we now can bound this middle term by two times the right-side function. This means that $(x + y)^2 \leq 3(x^2 + y^2)$, and so the result holds. ∎

2.3 Growth Rates and Dominance Relations

With the Big Oh notation, we cavalierly discard the multiplicative constants. Thus, the functions $f(n) = 0.001n^2$ and $g(n) = 1000n^2$ are treated identically, even though $g(n)$ is a million times larger than $f(n)$ for all values of n.

n $f(n)$	$\lg n$	n	$n \lg n$	n^2	2^n	$n!$
10	0.003 μs	0.01 μs	0.033 μs	0.1 μs	1 μs	3.63 ms
20	0.004 μs	0.02 μs	0.086 μs	0.4 μs	1 ms	77.1 years
30	0.005 μs	0.03 μs	0.147 μs	0.9 μs	1 sec	8.4×10^{15} yrs
40	0.005 μs	0.04 μs	0.213 μs	1.6 μs	18.3 min	
50	0.006 μs	0.05 μs	0.282 μs	2.5 μs	13 days	
100	0.007 μs	0.1 μs	0.644 μs	10 μs	4×10^{13} yrs	
1,000	0.010 μs	1.00 μs	9.966 μs	1 ms		
10,000	0.013 μs	10 μs	130 μs	100 ms		
100,000	0.017 μs	0.10 ms	1.67 ms	10 sec		
1,000,000	0.020 μs	1 ms	19.93 ms	16.7 min		
10,000,000	0.023 μs	0.01 sec	0.23 sec	1.16 days		
100,000,000	0.027 μs	0.10 sec	2.66 sec	115.7 days		
1,000,000,000	0.030 μs	1 sec	29.90 sec	31.7 years		

Figure 2.4: Growth rates of common functions measured in nanoseconds

The reason why we are content with coarse Big Oh analysis is provided by Figure 2.4, which shows the growth rate of several common time analysis functions. In particular, it shows how long algorithms that use $f(n)$ operations take to run on a fast computer, where each operation takes one nanosecond (10^{-9} seconds). The following conclusions can be drawn from this table:

- All such algorithms take roughly the same time for $n = 10$.
- Any algorithm with $n!$ running time becomes useless for $n \geq 20$.
- Algorithms whose running time is 2^n have a greater operating range, but become impractical for $n > 40$.
- Quadratic-time algorithms whose running time is n^2 remain usable up to about $n = 10,000$, but quickly deteriorate with larger inputs. They are likely to be hopeless for $n >$ 1,000,000.
- Linear-time and $n \lg n$ algorithms remain practical on inputs of one billion items.
- An $O(\lg n)$ algorithm hardly breaks a sweat for any imaginable value of n.

The bottom line is that even ignoring constant factors, we get an excellent idea of whether a given algorithm is appropriate for a problem of a given size. An algorithm whose running time is $f(n) = n^3$ seconds will beat one whose running time is $g(n) =$ 1,000,000 $\cdot n^2$ seconds only when $n <$ 1,000,000. Such enormous differences in constant factors between algorithms occur far less frequently in practice than large problems do.

2.3.1 Dominance Relations

The Big Oh notation groups functions into a set of classes, such that all the functions in a particular class are equivalent with respect to the Big Oh. Functions $f(n) = 0.34n$ and $g(n) = 234{,}234n$ belong in the same class, namely those that are order $\Theta(n)$. Further, when two functions f and g belong to different classes, they are *different* with respect to our notation. Either $f(n) = O(g(n))$ or $g(n) = O(f(n))$, but not both.

We say that a faster-growing function *dominates* a slower-growing one, just as a faster-growing country eventually comes to dominate the laggard. When f and g belong to different classes (i.e., $f(n) \neq \Theta(g(n))$), we say g *dominates* f when $f(n) = O(g(n))$, sometimes written $g \gg f$.

The good news is that only a few function classes tend to occur in the course of basic algorithm analysis. These suffice to cover almost all the algorithms we will discuss in this text, and are listed in order of increasing dominance:

- *Constant functions,* $f(n) = 1$ – Such functions might measure the cost of adding two numbers, printing out "The Star Spangled Banner," or the growth realized by functions such as $f(n) = \min(n, 100)$. In the big picture, there is no dependence on the parameter n.
- *Logarithmic functions,* $f(n) = \log n$ – Logarithmic time-complexity shows up in algorithms such as binary search. Such functions grow quite slowly as n gets big, but faster than the constant function (which is standing still, after all). Logarithms will be discussed in more detail in Section 2.6 (page 46)
- *Linear functions,* $f(n) = n$ – Such functions measure the cost of looking at each item once (or twice, or ten times) in an n-element array, say to identify the biggest item, the smallest item, or compute the average value.
- *Superlinear functions,* $f(n) = n \lg n$ – This important class of functions arises in such algorithms as Quicksort and Mergesort. They grow just a little faster than linear (see Figure 2.4), just enough to be a different dominance class.
- *Quadratic functions,* $f(n) = n^2$ – Such functions measure the cost of looking at most or all *pairs* of items in an n-element universe. This arises in algorithms such as insertion sort and selection sort.
- *Cubic functions,* $f(n) = n^3$ – Such functions enumerate through all *triples* of items in an n-element universe. These also arise in certain dynamic programming algorithms developed in Chapter 8.
- *Exponential functions,* $f(n) = c^n$ *for a given constant* $c > 1$ – Functions like 2^n arise when enumerating all subsets of n items. As we have seen, exponential algorithms become useless fast, but not as fast as...
- *Factorial functions,* $f(n) = n!$ – Functions like $n!$ arise when generating all permutations or orderings of n items.

The intricacies of dominance relations will be futher discussed in Section 2.9.2 (page 56). However, all you really need to understand is that:

$$n! \gg 2^n \gg n^3 \gg n^2 \gg n \log n \gg n \gg \log n \gg 1$$

Take-Home Lesson: Although esoteric functions arise in advanced algorithm analysis, a small variety of time complexities suffice and account for most algorithms that are widely used in practice.

2.4 Working with the Big Oh

You learned how to do simplifications of algebraic expressions back in high school. Working with the Big Oh requires dusting off these tools. *Most* of what you learned there still holds in working with the Big Oh, but not everything.

2.4.1 Adding Functions

The sum of two functions is governed by the dominant one, namely:

$$O(f(n)) + O(g(n)) \to O(\max(f(n), g(n)))$$

$$\Omega(f(n)) + \Omega(g(n)) \to \Omega(\max(f(n), g(n)))$$

$$\Theta(f(n)) + \Theta(g(n)) \to \Theta(\max(f(n), g(n)))$$

This is very useful in simplifying expressions, since it implies that $n^3 + n^2 + n + 1 = O(n^3)$. Everything is small potatoes besides the dominant term.

The intuition is as follows. At least half the bulk of $f(n) + g(n)$ must come from the larger value. The dominant function will, by definition, provide the larger value as $n \to \infty$. Thus, dropping the smaller function from consideration reduces the value by at most a factor of $1/2$, which is just a multiplicative constant. Suppose $f(n) = O(n^2)$ and $g(n) = O(n^2)$. This implies that $f(n) + g(n) = O(n^2)$ as well.

2.4.2 Multiplying Functions

Multiplication is like repeated addition. Consider multiplication by any constant $c > 0$, be it 1.02 or 1,000,000. Multiplying a function by a constant can not affect its asymptotic behavior, because we can multiply the bounding constants in the Big Oh analysis of $c \cdot f(n)$ by $1/c$ to give appropriate constants for the Big Oh analysis of $f(n)$. Thus:

$$O(c \cdot f(n)) \to O(f(n))$$

$$\Omega(c \cdot f(n)) \to \Omega(f(n))$$

$$\Theta(c \cdot f(n)) \rightarrow \Theta(f(n))$$

Of course, c must be strictly positive (i.e., $c > 0$) to avoid any funny business, since we can wipe out even the fastest growing function by multiplying it by zero.

On the other hand, when two functions in a product are increasing, both are important. The function $O(n! \log n)$ dominates $n!$ just as much as $\log n$ dominates 1. In general,

$$O(f(n)) * O(g(n)) \rightarrow O(f(n) * g(n))$$

$$\Omega(f(n)) * \Omega(g(n)) \rightarrow \Omega(f(n) * g(n))$$

$$\Theta(f(n)) * \Theta(g(n)) \rightarrow \Theta(f(n) * g(n))$$

Stop and Think: Transitive Experience

Problem: Show that Big Oh relationships are transitive. That is, if $f(n) = O(g(n))$ and $g(n) = O(h(n))$, then $f(n) = O(h(n))$.

Solution: We always go back to the definition when working with the Big Oh. What we need to show here is that $f(n) \leq c_3 h(n)$ for $n > n_3$ given that $f(n) \leq c_1 g(n)$ and $g(n) \leq c_2 h(n)$, for $n > n_1$ and $n > n_2$, respectively. Cascading these inequalities, we get that

$$f(n) \leq c_1 g(n) \leq c_1 c_2 h(n)$$

for $n > n_3 = \max(n_1, n_2)$. ∎

2.5 Reasoning About Efficiency

Gross reasoning about an algorithm's running time of is usually easy given a precise written description of the algorithm. In this section, I will work through several examples, perhaps in greater detail than necessary.

2.5.1 Selection Sort

Here we analyze the selection sort algorithm, which repeatedly identifies the smallest remaining unsorted element and puts it at the end of the sorted portion of the array. An animation of selection sort in action appears in Figure 2.5, and the code is shown below:

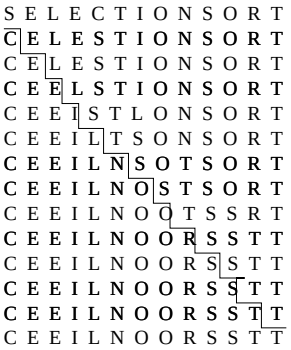

Figure 2.5: Animation of selection sort in action

```
selection_sort(int s[], int n)
{
        int i,j;                /* counters */
        int min;                /* index of minimum */

        for (i=0; i<n; i++) {
                min=i;
                for (j=i+1; j<n; j++)
                        if (s[j] < s[min]) min=j;
                swap(&s[i],&s[min]);
        }
}
```

The outer loop goes around n times. The nested inner loop goes around $n-i-1$ times, where i is the index of the outer loop. The exact number of times the *if* statement is executed is given by:

$$S(n) = \sum_{i=0}^{n-1} \sum_{j=i+1}^{n-1} 1 = \sum_{i=0}^{n-1} n - i - 1$$

What this sum is doing is adding up the integers in decreasing order starting from $n-1$, i.e.

$$S(n) = (n-1) + (n-2) + (n-3) + \ldots + 2 + 1$$

How can we reason about such a formula? We must solve the summation formula using the techniques of Section 1.3.5 (page 17) to get an exact value. But, with the Big Oh we are only interested in the *order* of the expression. One way to think about it is that we are adding up $n-1$ terms, whose average value is about $n/2$. This yields $S(n) \approx n(n-1)/2$.

Another way to think about it is in terms of upper and lower bounds. We have n terms at most, each of which is at most $n-1$. Thus, $S(n) \leq n(n-1) = O(n^2)$. We have $n/2$ terms each that are bigger than $n/2$. Thus $S(n) =\geq (n/2) \times (n/2) = \Omega(n^2)$. Together, this tells us that the running time is $\Theta(n^2)$, meaning that selection sort is quadratic.

2.5.2 Insertion Sort

A basic rule of thumb in Big Oh analysis is that worst-case running time follows from multiplying the largest number of times each nested loop can iterate. Consider the insertion sort algorithm presented on page 4, whose inner loops are repeated here:

```
for (i=1; i<n; i++) {
        j=i;
        while ((j>0) && (s[j] < s[j-1])) {
                swap(&s[j],&s[j-1]);
                j = j-1;
        }
}
```

How often does the inner *while* loop iterate? This is tricky because there are two different stopping conditions: one to prevent us from running off the bounds of the array ($j > 0$) and the other to mark when the element finds its proper place in sorted order ($s[j] < s[j-1]$). Since worst-case analysis seeks an upper bound on the running time, we ignore the early termination and assume that this loop *always* goes around i times. In fact, we can assume it *always* goes around n times since $i < n$. Since the outer loop goes around n times, insertion sort must be a quadratic-time algorithm, i.e. $O(n^2)$.

This crude "round it up" analysis always does the job, in that the Big Oh running time bound you get will always be correct. Occasionally, it might be too generous, meaning the actual worst case time might be of a lower order than implied by such analysis. Still, I strongly encourage this kind of reasoning as a basis for simple algorithm analysis.

2.5.3 String Pattern Matching

Pattern matching is the most fundamental algorithmic operation on text strings. This algorithm implements the find command available in any web browser or text editor:

Problem: Substring Pattern Matching
Input: A text string t and a pattern string p.
Output: Does t contain the pattern p as a substring, and if so where?

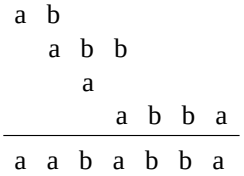

Figure 2.6: Searching for the substring *abba* in the text *aababba*.

Perhaps you are interested finding where "Skiena" appears in a given news article (well, I would be interested in such a thing). This is an instance of string pattern matching with t as the news article and p="Skiena."

There is a fairly straightforward algorithm for string pattern matching that considers the possibility that p may start at each possible position in t and then tests if this is so.

```
int findmatch(char *p, char *t)
{
        int i,j;                        /* counters */
        int m, n;                       /* string lengths */

        m = strlen(p);
        n = strlen(t);

        for (i=0; i<=(n-m); i=i+1) {
                j=0;
                while ((j<m) && (t[i+j]==p[j]))
                        j = j+1;
                if (j == m) return(i);
        }

        return(-1);
}
```

What is the worst-case running time of these two nested loops? The inner *while* loop goes around at most m times, and potentially far less when the pattern match fails. This, plus two other statements, lies within the outer *for* loop. The outer loop goes around at most $n - m$ times, since no complete alignment is possible once we get too far to the right of the text. The time complexity of nested loops multiplies, so this gives a worst-case running time of $O((n - m)(m + 2))$.

We did not count the time it takes to compute the length of the strings using the function *strlen*. Since the implementation of *strlen* is not given, we must guess how long it should take. If we explicitly count the number of characters until we

hit the end of the string; this would take time linear in the length of the string. This suggests that the running time should be $O(n + m + (n - m)(m + 2))$.

Let's use our knowledge of the Big Oh to simplify things. Since $m + 2 = \Theta(m)$, the "+2" isn't interesting, so we are left with $O(n + m + (n - m)m)$. Multiplying this out yields $O(n + m + nm - m^2)$, which still seems kind of ugly.

However, in any interesting problem we know that $n \geq m$, since it is impossible to have p as a substring of t for any pattern longer than the text itself. One consequence of this is that $n + m \leq 2n = \Theta(n)$. Thus our worst-case running time simplifies further to $O(n + nm - m^2)$.

Two more observations and we are done. First, note that $n \leq nm$, since $m \geq 1$ in any interesting pattern. Thus $n + nm = \Theta(nm)$, and we can drop the additive n, simplifying our analysis to $O(nm - m^2)$.

Finally, observe that the $-m^2$ term is negative, and thus only serves to lower the value within. Since the Big Oh gives an upper bound, we can drop any negative term without invalidating the upper bound. That $n \geq m$ implies that $mn \geq m^2$, so the negative term is not big enough to cancel any other term which is left. Thus we can simply express the worst-case running time of this algorithm as $O(nm)$.

After you get enough experience, you will be able to do such an algorithm analysis in your head without even writing the algorithm down. After all, algorithm design for a given task involves mentally rifling through different possibilities and selecting the best approach. This kind of fluency comes with practice, but if you are confused about why a given algorithm runs in $O(f(n))$ time, start by writing it out carefully and then employ the reasoning we used in this section.

2.5.4 Matrix Multiplication

Nested summations often arise in the analysis of algorithms with nested loops. Consider the problem of matrix multiplication:

Problem: Matrix Multiplication
Input: Two matrices, A (of dimension $x \times y$) and B (dimension $y \times z$).
Output: An $x \times z$ matrix C where $C[i][j]$ is the dot product of the ith row of A and the jth column of B.

Matrix multiplication is a fundamental operation in linear algebra, presented with an example in catalog in Section 13.3 (page 401). That said, the elementary algorithm for matrix multiplication is implemented as a tight product of three nested loops:

```
for (i=1; i<=x; i++)
        for (j=1; j<=y; j++) {
                C[i][j] = 0;
                for (k=1; k<=z; k++)
                        C[i][j] += A[i][k] * B[k][j];
        }
```

How can we analyze the time complexity of this algorithm? The number of multiplications $M(x, y, z)$ is given by the following summation:

$$M(x, y, z) = \sum_{i=1}^{x} \sum_{j=1}^{y} \sum_{k=1}^{z} 1$$

Sums get evaluated from the right inward. The sum of z ones is z, so

$$M(x, y, z) = \sum_{i=1}^{x} \sum_{j=1}^{y} z$$

The sum of y zs is just as simple, yz, so

$$M(x, y, z) = \sum_{i=1}^{x} yz$$

Finally, the sum of x yzs is xyz.

Thus the running of this matrix multiplication algorithm is $O(xyz)$. If we consider the common case where all three dimensions are the same, this becomes $O(n^3)$—i.e. , a cubic algorithm.

2.6 Logarithms and Their Applications

Logarithm is an anagram of algorithm, but that's not why we need to know what logarithms are. You've seen the button on your calculator but may have forgotten why it is there. A *logarithm* is simply an inverse exponential function. Saying $b^x = y$ is equivalent to saying that $x = \log_b y$. Further, this definition is the same as saying $b^{\log_b y} = y$.

Exponential functions grow at a distressingly fast rate, as anyone who has ever tried to pay off a credit card balance understands. Thus, inverse exponential functions—i.e. logarithms—grow refreshingly slowly. Logarithms arise in any process where things are repeatedly halved. We now look at several examples.

2.6.1 Logarithms and Binary Search

Binary search is a good example of an $O(\log n)$ algorithm. To locate a particular person p in a telephone book containing n names, you start by comparing p against the middle, or $(n/2)$nd name, say *Monroe, Marilyn*. Regardless of whether p belongs before this middle name (*Dean, James*) or after it (*Presley, Elvis*), after only one comparison you can discard one half of all the names in the book. The number of steps the algorithm takes equals the number of times we can halve n until only one name is left. By definition, this is exactly $\log_2 n$. Thus, twenty comparisons suffice to find any name in the million-name Manhattan phone book!

Binary search is one of the most powerful ideas in algorithm design. This power becomes apparent if we imagine being forced to live in a world with only unsorted

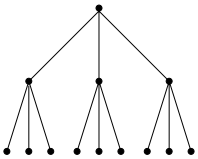

Figure 2.7: A height h tree with d children per node as d^h leaves. Here $h = 2$ and $d = 3$

telephone books. Figure 2.4 shows that $O(\log n)$ algorithms are fast enough to be used on problem instances of essentially unlimited size.

2.6.2 Logarithms and Trees

A binary tree of height 1 can have up to 2 leaf nodes, while a tree of height two can have up to four leaves. What is the height h of a rooted binary tree with n leaf nodes? Note that the number of leaves doubles every time we increase the height by one. To account for n leaves, $n = 2^h$ which implies that $h = \log_2 n$.

What if we generalize to trees that have d children, where $d = 2$ for the case of binary trees? A tree of height 1 can have up to d leaf nodes, while one of height two can have up to d^2 leaves. The number of possible leaves multiplies by d every time we increase the height by one, so to account for n leaves, $n = d^h$ which implies that $h = \log_d n$, as shown in Figure 2.7.

The punch line is that very short trees can have very many leaves, which is the main reason why binary trees prove fundamental to the design of fast data structures.

2.6.3 Logarithms and Bits

There are two bit patterns of length 1 (0 and 1) and four of length 2 (00, 01, 10, and 11). How many bits w do we need to represent any one of n different possibilities, be it one of n items or the integers from 1 to n?

The key observation is that there must be at least n different bit patterns of length w. Since the number of different bit patterns doubles as you add each bit, we need at least w bits where $2^w = n$—i.e., we need $w = \log_2 n$ bits.

2.6.4 Logarithms and Multiplication

Logarithms were particularly important in the days before pocket calculators. They provided the easiest way to multiply big numbers by hand, either implicitly using a slide rule or explicitly by using a book of logarithms.

Logarithms are still useful for multiplication, particularly for exponentiation. Recall that $\log_a(xy) = \log_a(x) + \log_a(y)$; i.e. , the log of a product is the sum of the logs. A direct consequence of this is

$$\log_a n^b = b \cdot \log_a n$$

So how can we compute a^b for any a and b using the $\exp(x)$ and $\ln(x)$ functions on your calculator, where $\exp(x) = e^x$ and $\ln(x) = \log_e(x)$? We know

$$a^b = \exp(\ln(a^b)) = \exp(b \ln a)$$

so the problem is reduced to one multiplication plus one call to each of these functions.

2.6.5 Fast Exponentiation

Suppose that we need to *exactly* compute the value of a^n for some reasonably large n. Such problems occur in primality testing for cryptography, as discussed in Section 13.8 (page 420). Issues of numerical precision prevent us from applying the formula above.

The simplest algorithm performs $n - 1$ multiplications, by computing $a \times a \times \ldots \times a$. However, we can do better by observing that $n = \lfloor n/2 \rfloor + \lceil n/2 \rceil$. If n is even, then $a^n = (a^{n/2})^2$. If n is odd, then $a^n = a(a^{\lfloor n/2 \rfloor})^2$. In either case, we have halved the size of our exponent at the cost of, at most, two multiplications, so $O(\lg n)$ multiplications suffice to compute the final value.

```
function power(a, n)
    if (n = 0) return(1)
    x = power(a, ⌊n/2⌋)
    if (n is even) then return(x^2)
        else return(a × x^2)
```

This simple algorithm illustrates an important principle of divide and conquer. It always pays to divide a job as evenly as possible. This principle applies to real life as well. When n is not a power of two, the problem cannot always be divided perfectly evenly, but a difference of one element between the two sides cannot cause any serious imbalance.

2.6.6 Logarithms and Summations

The *Harmonic numbers* arise as a special case of arithmetic progression, namely $H(n) = S(n, -1)$. They reflect the sum of the progression of simple reciprocals, namely,

$$H(n) = \sum_{i=1}^{n} 1/i \sim \ln n$$

Loss (apply the greatest)	Increase in level
(A) $2,000 or less	no increase
(B) More than $2,000	add 1
(C) More than $5,000	add 2
(D) More than $10,000	add 3
(E) More than $20,000	add 4
(F) More than $40,000	add 5
(G) More than $70,000	add 6
(H) More than $120,000	add 7
(I) More than $200,000	add 8
(J) More than $350,000	add 9
(K) More than $500,000	add 10
(L) More than $800,000	add 11
(M) More than $1,500,000	add 12
(N) More than $2,500,000	add 13
(O) More than $5,000,000	add 14
(P) More than $10,000,000	add 15
(Q) More than $20,000,000	add 16
(R) More than $40,000,000	add 17
(Q) More than $80,000,000	add 18

Figure 2.8: The Federal Sentencing Guidelines for fraud

The Harmonic numbers prove important because they usually explain "where the log comes from" when one magically pops out from algebraic manipulation. For example, the key to analyzing the average case complexity of Quicksort is the summation $S(n) = n \sum_{i=1}^{n} 1/i$. Employing the Harmonic number identity immediately reduces this to $\Theta(n \log n)$.

2.6.7 Logarithms and Criminal Justice

Figure 2.8 will be our final example of logarithms in action. This table appears in the Federal Sentencing Guidelines, used by courts throughout the United States. These guidelines are an attempt to standardize criminal sentences, so that a felon convicted of a crime before one judge receives the same sentence that they would before a different judge. To accomplish this, the judges have prepared an intricate point function to score the depravity of each crime and map it to time-to-serve.

Figure 2.8 gives the actual point function for fraud—a table mapping dollars stolen to points. Notice that the punishment increases by one level each time the amount of money stolen roughly doubles. That means that the level of punishment (which maps roughly linearly to the amount of time served) grows logarithmically with the amount of money stolen.

Think for a moment about the consequences of this. Many a corrupt CEO certainly has. It means that your total sentence grows *extremely* slowly with the amount of money you steal. Knocking off five liquor stores for $10,000 each will get you more time than embezzling $1,000,000 once. The corresponding benefit of stealing really large amounts of money is even greater. The moral of logarithmic growth is clear: *"If you are gonna do the crime, make it worth the time!"*

Take-Home Lesson: Logarithms arise whenever things are repeatedly halved or doubled.

2.7 Properties of Logarithms

As we have seen, stating $b^x = y$ is equivalent to saying that $x = \log_b y$. The b term is known as the *base* of the logarithm. Three bases are of particular importance for mathematical and historical reasons:

- *Base* $b = 2$ – The *binary logarithm*, usually denoted $\lg x$, is a base 2 logarithm. We have seen how this base arises whenever repeated halving (i.e., binary search) or doubling (i.e., nodes in trees) occurs. Most algorithmic applications of logarithms imply binary logarithms.

- *Base* $b = e$ – The *natural log*, usually denoted $\ln x$, is a base $e = 2.71828\ldots$ logarithm. The inverse of $\ln x$ is the exponential function $\exp(x) = e^x$ on your calculator. Thus, composing these functions gives us

$$\exp(\ln x) = x$$

- *Base* $b = 10$ – Less common today is the base-10 or *common logarithm*, usually denoted as $\log x$. This base was employed in slide rules and logarithm books in the days before pocket calculators.

We have already seen one important property of logarithms, namely that

$$\log_a(xy) = \log_a(x) + \log_a(y)$$

The other important fact to remember is that it is easy to convert a logarithm from one base to another. This is a consequence of the formula:

$$\log_a b = \frac{\log_c b}{\log_c a}$$

Thus, changing the base of $\log b$ from base-a to base-c simply involves dividing by $\log_c a$. It is easy to convert a common log function to a natural log function, and vice versa.

Two implications of these properties of logarithms are important to appreciate from an algorithmic perspective:

- *The base of the logarithm has no real impact on the growth rate-* Compare the following three values: $\log_2(1,000,000) = 19.9316$, $\log_3(1,000,000) = 12.5754$, and $\log_{100}(1,000,000) = 3$. A big change in the base of the logarithm produces little difference in the value of the log. Changing the base of the log from a to c involves dividing by $\log_c a$. This conversion factor is lost to the Big Oh notation whenever a and c are constants. Thus we are usually justified in ignoring the base of the logarithm when analyzing algorithms.

- *Logarithms cut any function down to size-* The growth rate of the logarithm of any polynomial function is $O(\lg n)$. This follows because

  $$\log_a n^b = b \cdot \log_a n$$

  The power of binary search on a wide range of problems is a consequence of this observation. Note that doing a binary search on a sorted array of n^2 things requires only twice as many comparisons as a binary search on n things.

  Logarithms efficiently cut any function down to size. It is hard to do arithmetic on factorials except for logarithms, since

  $$n! = \Pi_{i=1}^{n} i \rightarrow \log n! = \sum_{i=1}^{n} \log i = \Theta(n \log n)$$

  provides another way for logarithms to pop up in algorithm analysis.

Stop and Think: Importance of an Even Split

Problem: How many queries does binary search take on the million-name Manhattan phone book if each split was 1/3 to 2/3 instead of 1/2 to 1/2?

Solution: When performing binary searches in a telephone book, how important is it that each query split the book exactly in half? Not much. For the Manhattan telephone book, we now use $\log_{3/2}(1,000,000) \approx 35$ queries in the worst case, not a significant change from $\log_2(1,000,000) \approx 20$. The power of binary search comes from its logarithmic complexity, not the base of the log. ∎

2.8 War Story: Mystery of the Pyramids

That look in his eyes should have warned me even before he started talking.

"We want to use a parallel supercomputer for a numerical calculation up to 1,000,000,000, but we need a faster algorithm to do it."

I'd seen that distant look before. Eyes dulled from too much exposure to the raw horsepower of supercomputers—machines so fast that brute force seemed to eliminate the need for clever algorithms; at least until the problems got hard enough.

"I am working with a Nobel prize winner to use a computer on a famous problem in number theory. Are you familiar with Waring's problem?"

I knew some number theory. "Sure. Waring's problem asks whether every integer can be expressed at least one way as the sum of at most four integer squares. For example, $78 = 8^2 + 3^2 + 2^2 + 1^2 = 7^2 + 5^2 + 2^2$. I remember proving that four squares suffice to represent any integer in my undergraduate number theory class. Yes, it's a famous problem but one that got solved about 200 years ago."

"No, we are interested in a different version of Waring's problem. A *pyramidal number* is a number of the form $(m^3 - m)/6$, for $m \geq 2$. Thus the first several pyramidal numbers are 1, 4, 10, 20, 35, 56, 84, 120, and 165. The conjecture since 1928 is that every integer can be represented by the sum of at most five such pyramidal numbers. We want to use a supercomputer to prove this conjecture on all numbers from 1 to 1,000,000,000."

"Doing a billion of anything will take a substantial amount of time," I warned. "The time you spend to compute the minimum representation of each number will be critical, because you are going to do it one billion times. Have you thought about what kind of an algorithm you are going to use?"

"We have already written our program and run it on a parallel supercomputer. It works very fast on smaller numbers. Still, it takes much too much time as soon as we get to 100,000 or so."

Terrific, I thought. Our supercomputer junkie had discovered asymptotic growth. No doubt his algorithm ran in something like quadratic time, and he got burned as soon as n got large.

"We need a faster program in order to get to one billion. Can you help us? Of course, we can run it on our parallel supercomputer when you are ready."

I am a sucker for this kind of challenge, finding fast algorithms to speed up programs. I agreed to think about it and got down to work.

I started by looking at the program that the other guy had written. He had built an array of all the $\Theta(n^{1/3})$ pyramidal numbers from 1 to n inclusive.[2] To test each number k in this range, he did a brute force test to establish whether it was the sum of two pyramidal numbers. If not, the program tested whether it was the sum of three of them, then four, and finally five, until it first got an answer. About 45% of the integers are expressible as the sum of three pyramidal numbers. Most of the remaining 55% require the sum of four, and usually each of these can be represented in many different ways. Only 241 integers are known to require the sum of five pyramidal numbers, the largest being 343,867. For about half of the n numbers, this algorithm presumably went through all of the three-tests and at least

[2]Why $n^{1/3}$? Recall that pyramidal numbers are of the form $(m^3 - m)/6$. The largest m such that the resulting number is at most n is roughly $\sqrt[3]{6n}$, so there are $\Theta(n^{1/3})$ such numbers.

some of the four-tests before terminating. Thus, the total time for this algorithm would be at least $O(n \times (n^{1/3})^3) = O(n^2)$ time, where $n = 1{,}000{,}000{,}000$. No wonder his program cried "Uncle."

Anything that was going to do significantly better on a problem this large had to avoid explicitly testing all triples. For each value of k, we were seeking the smallest set of pyramidal numbers that add up to exactly to k. This problem is called the *knapsack problem*, and is discussed in Section 13.10 (page 427). In our case, the weights are the set of pyramidal numbers no greater than n, with an additional constraint that the knapsack holds exactly k items.

A standard approach to solving knapsack precomputes the sum of smaller subsets of the items for use in computing larger subsets. If we have a table of all sums of two numbers and want to know whether k is expressible as the sum of three numbers, we can ask whether k is expressible as the sum of a single number plus a number in this two-table.

Therefore I needed a table of all integers less than n that can be expressed as the sum of two of the 1,818 pyramidal numbers less than 1,000,000,000. There can be at most $1,818^2 = 3{,}305{,}124$ of them. Actually, there are only about half this many after we eliminate duplicates and any sum bigger than our target. Building a sorted array storing these numbers would be no big deal. Let's call this sorted data structure of all pair-sums the *two*-table.

To find the minimum decomposition for a given k, I would first check whether it was one of the 1,818 pyramidal numbers. If not, I would then check whether k was in the sorted table of the sums of two pyramidal numbers. To see whether k was expressible as the sum of three such numbers, all I had to do was check whether $k - p[i]$ was in the *two*-table for $1 \leq i \leq 1{,}818$. This could be done quickly using binary search. To see whether k was expressible as the sum of four pyramidal numbers, I had to check whether $k - two[i]$ was in the two-table for any $1 \leq i \leq |two|$. However, since almost every k was expressible in many ways as the sum of four pyramidal numbers, this test would terminate quickly, and the total time taken would be dominated by the cost of the threes. Testing whether k was the sum of three pyramidal numbers would take $O(n^{1/3} \lg n)$. Running this on each of the n integers gives an $O(n^{4/3} \lg n)$ algorithm for the complete job. Comparing this to his $O(n^2)$ algorithm for $n = 1{,}000{,}000{,}000$ suggested that my algorithm was a cool *30,000* times faster than his original!

My first attempt to code this solved up to $n = 1,000,000$ on my ancient Sparc ELC in about 20 minutes. From here, I experimented with different data structures to represent the sets of numbers and different algorithms to search these tables. I tried using hash tables and bit vectors instead of sorted arrays, and experimented with variants of binary search such as interpolation search (see Section 14.2 (page 441)). My reward for this work was solving up to n =1,000,000 in under three minutes, a factor of six improvement over my original program.

With the real thinking done, I worked to tweak a little more performance out of the program. I avoided doing a sum-of-four computation on any k when $k - 1$ was

the sum-of-three, since 1 is a pyramidal number, saving about 10% of the total run time using this trick alone. Finally, I got out my profiler and tried some low-level tricks to squeeze a little more performance out of the code. For example, I saved another 10% by replacing a single procedure call with in line code.

At this point, I turned the code over to the supercomputer guy. What he did with it is a depressing tale, which is reported in Section 7.10 (page 268).

In writing up this war story, I went back to rerun my program more than ten years later. On my desktop SunBlade 150, getting to 1,000,000 now took 27.0 seconds using the gcc compiler without turning on any compiler optimization. With Level 4 optimization, the job ran in just 14.0 seconds—quite a tribute to the quality of the optimizer. The run time on my desktop machine improved by a factor of about three over the four-year period prior to my first edition of this book, with an additional 5.3 times over the last 11 years. These speedups are probably typical for most desktops.

The primary lesson of this war story is to show the enormous potential for algorithmic speedups, as opposed to the fairly limited speedup obtainable via more expensive hardware. I sped his program up by about 30,000 times. His million-dollar computer had 16 processors, each reportedly five times faster on integer computations than the $3,000 machine on my desk. That gave a maximum potential speedup of less than 100 times. Clearly, the algorithmic improvement was the big winner here, as it is certain to be in any sufficiently large computation.

2.9 Advanced Analysis (*)

Ideally, each of us would be fluent in working with the mathematical techniques of asymptotic analysis. And ideally, each of us would be rich and good looking as well.

In this section I will survey the major techniques and functions employed in advanced algorithm analysis. I consider this optional material—it will not be used elsewhere in the textbook section of this book. That said, it will make some of the complexity functions reported in the Hitchhiker's Guide far less mysterious.

2.9.1 Esoteric Functions

The bread-and-butter classes of complexity functions were presented in Section 2.3.1 (page 39). More esoteric functions also make appearances in advanced algorithm analysis. Although we will not see them much in this book, it is still good business to know what they mean and where they come from:

- *Inverse Ackerman's function* $f(n) = \alpha(n)$ – This function arises in the detailed analysis of several algorithms, most notably the Union-Find data structure discussed in Section 6.1.3 (page 198).

  The exact definition of this function and why it arises will not be discussed further. It is sufficient to think of it as geek talk for the slowest-growing

complexity function. Unlike the constant function $f(n) = 1$, it eventually gets to infinity as $n \to \infty$, but it certainly takes its time about it. The value of $\alpha(n) < 5$ for any value of n that can be written in this physical universe.

- $f(n) = \log \log n$ – The "log log" function is just that—the logarithm of the logarithm of n. One natural example of how it might arise is doing a binary search on a sorted array of only $\lg n$ items.

- $f(n) = \log n / \log \log n$ – This function grows a little slower than $\log n$ because it is divided by an even slower growing function.

  To see where this arises, consider an n-leaf rooted tree of degree d. For binary trees, i.e. when $d = 2$, the height h is given

  $$n = 2^h \to h = \lg n$$

  by taking the logarithm of both sides of the equation. Now consider the height of such a tree when the degree $d = \log n$. Then

  $$n = (\log n)^h \to h = \log n / \log \log n$$

- $f(n) = \log^2 n$ – This is the product of log functions—i.e., $(\log n) \times (\log n)$. It might arise if we wanted to count the bits looked at in doing a binary search on n items, each of which was an integer from 1 to (say) n^2. Each such integer requires a $\lg(n^2) = 2 \lg n$ bit representation, and we look at $\lg n$ of them, for a total of $2 \lg^2 n$ bits.

  The "log squared" function typically arises in the design of intricate nested data structures, where each node in (say) a binary tree represents another data structure, perhaps ordered on a different key.

- $f(n) = \sqrt{n}$ – The square root is not so esoteric, but represents the class of "sublinear polynomials" since $\sqrt{n} = n^{1/2}$. Such functions arise in building d-dimensional grids that contain n points. A $\sqrt{n} \times \sqrt{n}$ square has area n, and an $n^{1/3} \times n^{1/3} \times n^{1/3}$ cube has volume n. In general, a d-dimensional hypercube of length $n^{1/d}$ on each side has volume d.

- $f(n) = n^{(1+\epsilon)}$ – Epsilon (ϵ) is the mathematical symbol to denote a constant that can be made arbitrarily small but never quite goes away.

  It arises in the following way. Suppose I design an algorithm that runs in $2^c n^{(1+1/c)}$ time, and I get to pick whichever c I want. For $c = 2$, this is $4n^{3/2}$ or $O(n^{3/2})$. For $c = 3$, this is $8n^{4/3}$ or $O(n^{4/3})$, which is better. Indeed, the exponent keeps getting better the larger I make c.

  The problem is that I cannot make c arbitrarily large before the 2^c term begins to dominate. Instead, we report this algorithm as running in $O(n^{1+\epsilon})$, and leave the best value of ϵ to the beholder.

2.9.2 Limits and Dominance Relations

The dominance relation between functions is a consequence of the theory of limits, which you may recall from Calculus. We say that $f(n)$ *dominates* $g(n)$ if $\lim_{n\to\infty} g(n)/f(n) = 0$.

Let's see this definition in action. Suppose $f(n) = 2n^2$ and $g(n) = n^2$. Clearly $f(n) > g(n)$ for all n, but it does not dominate since

$$\lim_{n\to\infty} g(n)/f(n) = \lim_{n\to\infty} n^2/2n^2 = \lim_{n\to\infty} 1/2 \neq 0$$

This is to be expected because both functions are in the class $\Theta(n^2)$. What about $f(n) = n^3$ and $g(n) = n^2$? Since

$$\lim_{n\to\infty} g(n)/f(n) = \lim_{n\to\infty} n^2/n^3 = \lim_{n\to\infty} 1/n = 0$$

the higher-degree polynomial dominates. This is true for any two polynomials, namely that n^a dominates n^b if $a > b$ since

$$\lim_{n\to\infty} n^b/n^a = \lim_{n\to\infty} n^{b-a} \to 0$$

Thus $n^{1.2}$ dominates $n^{1.1999999}$.

Now consider two exponential functions, say $f(n) = 3^n$ and $g(n) = 2^n$. Since

$$\lim_{n\to\infty} g(n)/f(n) = 2^n/3^n = \lim_{n\to\infty} (2/3)^n = 0$$

the exponential with the higher base dominates.

Our ability to prove dominance relations from scratch depends upon our ability to prove limits. Let's look at one important pair of functions. Any polynomial (say $f(n) = n^\epsilon$) dominates logarithmic functions (say $g(n) = \lg n$). Since $n = 2^{\lg n}$,

$$f(n) = (2^{\lg n})^\epsilon = 2^{\epsilon \lg n}$$

Now consider

$$\lim_{n\to\infty} g(n)/f(n) = \lg n/2^{\epsilon \lg n}$$

In fact, this does go to 0 as $n \to \infty$.

Take-Home Lesson: By interleaving the functions here with those of Section 2.3.1 (page 39), we see where everything fits into the dominance pecking order:

$$n! \gg c^n \gg n^3 \gg n^2 \gg n^{1+\epsilon} \gg n \log n \gg n \gg \sqrt{n} \gg$$
$$\log^2 n \gg \log n \gg \log n/\log\log n \gg \log\log n \gg \alpha(n) \gg 1$$

Chapter Notes

Most other algorithm texts devote considerably more efforts to the formal analysis of algorithms than we have here, and so we refer the theoretically-inclined reader

elsewhere for more depth. Algorithm texts more heavily stressing analysis include [CLRS01, KT06].

The book *Concrete Mathematics* by Knuth, Graham, and Patashnik [GKP89] offers an interesting and thorough presentation of mathematics for the analysis of algorithms. Niven and Zuckerman [NZ80] is an nice introduction to number theory, including Waring's problem, discussed in the war story.

The notion of dominance also gives rise to the "Little Oh" notation. We say that $f(n) = o(g(n))$ iff $g(n)$ dominates $f(n)$. Among other things, the Little Oh proves useful for asking questions. Asking for an $o(n^2)$ algorithm means you want one that is better than quadratic in the worst case—and means you would be willing to settle for $O(n^{1.999} \log^2 n)$.

2.10 Exercises

Program Analysis

2-1. *[3]* What value is returned by the following function? Express your answer as a function of n. Give the worst-case running time using the Big Oh notation.

```
function mystery(n)
    r := 0
    for i := 1 to n − 1 do
        for j := i + 1 to n do
            for k := 1 to j do
                r := r + 1
    return(r)
```

2-2. *[3]* What value is returned by the following function? Express your answer as a function of n. Give the worst-case running time using Big Oh notation.

```
function pesky(n)
    r := 0
    for i := 1 to n do
        for j := 1 to i do
            for k := j to i + j do
                r := r + 1
    return(r)
```

2-3. *[5]* What value is returned by the following function? Express your answer as a function of n. Give the worst-case running time using Big Oh notation.

```
function prestiferous(n)
    r := 0
    for i := 1 to n do
        for j := 1 to i do
            for k := j to i + j do
                for l := 1 to i + j − k do
```

```
                    r := r + 1
            return(r)
```

2-4. *[8]* What value is returned by the following function? Express your answer as a function of n. Give the worst-case running time using Big Oh notation.

```
function conundrum(n)
    r := 0
    for i := 1 to n do
      for j := i + 1 to n do
        for k := i + j − 1 to n do
            r := r + 1
    return(r)
```

2-5. *[5]* Suppose the following algorithm is used to evaluate the polynomial

$$p(x) = a_n x^n + a_{n-1} x^{n-1} + \ldots + a_1 x + a_0$$

```
p := a_0;
xpower := 1;
for i := 1 to n do
      xpower := x * xpower;
      p := p + a_i * xpower
end
```

(a) How many multiplications are done in the worst-case? How many additions?

(b) How many multiplications are done on the average?

(c) Can you improve this algorithm?

2-6. *[3]* Prove that the following algorithm for computing the maximum value in an array $A[1..n]$ is correct.

```
function max(A)
                    m := A[1]
                    for i := 2 to n do
                          if A[i] > m then m := A[i]
                    return (m)
```

Big Oh

2-7. *[3]* True or False?

(a) Is $2^{n+1} = O(2^n)$?

(b) Is $2^{2n} = O(2^n)$?

2-8. *[3]* For each of the following pairs of functions, either $f(n)$ is in $O(g(n))$, $f(n)$ is in $\Omega(g(n))$, or $f(n) = \Theta(g(n))$. Determine which relationship is correct and briefly explain why.

(a) $f(n) = \log n^2$; $g(n) = \log n + 5$

(b) $f(n) = \sqrt{n}$; $g(n) = \log n^2$

(c) $f(n) = \log^2 n$; $g(n) = \log n$

(d) $f(n) = n$; $g(n) = \log^2 n$

(e) $f(n) = n \log n + n$; $g(n) = \log n$

(f) $f(n) = 10$; $g(n) = \log 10$

(g) $f(n) = 2^n$; $g(n) = 10n^2$

(h) $f(n) = 2^n$; $g(n) = 3^n$

2-9. *[3]* For each of the following pairs of functions $f(n)$ and $g(n)$, determine whether $f(n) = O(g(n))$, $g(n) = O(f(n))$, or both.

(a) $f(n) = (n^2 - n)/2$, $g(n) = 6n$

(b) $f(n) = n + 2\sqrt{n}$, $g(n) = n^2$

(c) $f(n) = n \log n$, $g(n) = n\sqrt{n}/2$

(d) $f(n) = n + \log n$, $g(n) = \sqrt{n}$

(e) $f(n) = 2(\log n)^2$, $g(n) = \log n + 1$

(f) $f(n) = 4n \log n + n$, $g(n) = (n^2 - n)/2$

2-10. *[3]* Prove that $n^3 - 3n^2 - n + 1 = \Theta(n^3)$.

2-11. *[3]* Prove that $n^2 = O(2^n)$.

2-12. *[3]* For each of the following pairs of functions $f(n)$ and $g(n)$, give an appropriate positive constant c such that $f(n) \leq c \cdot g(n)$ for all $n > 1$.

(a) $f(n) = n^2 + n + 1$, $g(n) = 2n^3$

(b) $f(n) = n\sqrt{n} + n^2$, $g(n) = n^2$

(c) $f(n) = n^2 - n + 1$, $g(n) = n^2/2$

2-13. *[3]* Prove that if $f_1(n) = O(g_1(n))$ and $f_2(n) = O(g_2(n))$, then $f_1(n) + f_2(n) = O(g_1(n) + g_2(n))$.

2-14. *[3]* Prove that if $f_1(N) = \Omega(g_1(n))$ and $f_2(n) = \Omega(g_2(n))$, then $f_1(n) + f_2(n) = \Omega(g_1(n) + g_2(n))$.

2-15. *[3]* Prove that if $f_1(n) = O(g_1(n))$ and $f_2(n) = O(g_2(n))$, then $f_1(n) \cdot f_2(n) = O(g_1(n) \cdot g_2(n))$

2-16. *[5]* Prove for all $k \geq 1$ and all sets of constants $\{a_k, a_{k-1}, \ldots, a_1, a_0\} \in R$,

$$a_k n^k + a_{k-1} n^{k-1} + ... + a_1 n + a_0 = O(n^k)$$

2-17. *[5]* Show that for any real constants a and b, $b > 0$

$$(n + a)^b = \Theta(n^b)$$

2-18. *[5]* List the functions below from the lowest to the highest order. If any two or more are of the same order, indicate which.

n	2^n	$n \lg n$	$\ln n$
$n - n^3 + 7n^5$	$\lg n$	$\sqrt{n}$	e^n
$n^2 + \lg n$	n^2	2^{n-1}	$\lg \lg n$
n^3	$(\lg n)^2$	$n!$	$n^{1+\varepsilon}$ where $0 < \varepsilon < 1$

2-19. *[5]* List the functions below from the lowest to the highest order. If any two or more are of the same order, indicate which.

$\sqrt{n}$	n	2^n
$n \log n$	$n - n^3 + 7n^5$	$n^2 + \log n$
n^2	n^3	$\log n$
$n^{\frac{1}{3}} + \log n$	$(\log n)^2$	$n!$
$\ln n$	$\frac{n}{\log n}$	$\log \log n$
$(1/3)^n$	$(3/2)^n$	6

2-20. *[5]* Find two functions $f(n)$ and $g(n)$ that satisfy the following relationship. If no such f and g exist, write "None."

(a) $f(n) = o(g(n))$ and $f(n) \neq \Theta(g(n))$

(b) $f(n) = \Theta(g(n))$ and $f(n) = o(g(n))$

(c) $f(n) = \Theta(g(n))$ and $f(n) \neq O(g(n))$

(d) $f(n) = \Omega(g(n))$ and $f(n) \neq O(g(n))$

2-21. *[5]* True or False?

(a) $2n^2 + 1 = O(n^2)$

(b) $\sqrt{n} = O(\log n)$

(c) $\log n = O(\sqrt{n})$

(d) $n^2(1 + \sqrt{n}) = O(n^2 \log n)$

(e) $3n^2 + \sqrt{n} = O(n^2)$

(f) $\sqrt{n} \log n = O(n)$

(g) $\log n = O(n^{-1/2})$

2-22. *[5]* For each of the following pairs of functions $f(n)$ and $g(n)$, state whether $f(n) = O(g(n))$, $f(n) = \Omega(g(n))$, $f(n) = \Theta(g(n))$, or none of the above.

(a) $f(n) = n^2 + 3n + 4$, $g(n) = 6n + 7$

(b) $f(n) = n\sqrt{n}$, $g(n) = n^2 - n$

(c) $f(n) = 2^n - n^2$, $g(n) = n^4 + n^2$

2-23. *[3]* For each of these questions, briefly explain your answer.

(a) If I prove that an algorithm takes $O(n^2)$ worst-case time, is it possible that it takes $O(n)$ on some inputs?

(b) If I prove that an algorithm takes $O(n^2)$ worst-case time, is it possible that it takes $O(n)$ on all inputs?

(c) If I prove that an algorithm takes $\Theta(n^2)$ worst-case time, is it possible that it takes $O(n)$ on some inputs?

(d) If I prove that an algorithm takes $\Theta(n^2)$ worst-case time, is it possible that it takes $O(n)$ on all inputs?

(e) Is the function $f(n) = \Theta(n^2)$, where $f(n) = 100n^2$ for even n and $f(n) = 20n^2 - n\log_2 n$ for odd n?

2-24. *[3]* For each of the following, answer *yes*, *no*, or *can't tell*. Explain your reasoning.

(a) Is $3^n = O(2^n)$?

(b) Is $\log 3^n = O(\log 2^n)$?

(c) Is $3^n = \Omega(2^n)$?

(d) Is $\log 3^n = \Omega(\log 2^n)$?

2-25. *[5]* For each of the following expressions $f(n)$ find a simple $g(n)$ such that $f(n) = \Theta(g(n))$.

(a) $f(n) = \sum_{i=1}^{n} \frac{1}{i}$.

(b) $f(n) = \sum_{i=1}^{n} \lceil \frac{1}{i} \rceil$.

(c) $f(n) = \sum_{i=1}^{n} \log i$.

(d) $f(n) = \log(n!)$.

2-26. *[5]* Place the following functions into increasing asymptotic order.

$f_1(n) = n^2 \log_2 n$, $f_2(n) = n(\log_2 n)^2$, $f_3(n) = \sum_{i=0}^{n} 2^i$, $f_4(n) = \log_2(\sum_{i=0}^{n} 2^i)$.

2-27. *[5]* Place the following functions into increasing asymptotic order. If two or more of the functions are of the same asymptotic order then indicate this.

$f_1(n) = \sum_{i=1}^{n} \sqrt{i}$, $f_2(n) = (\sqrt{n}) \log n$, $f_3(n) = n\sqrt{\log n}$, $f_4(n) = 12n^{\frac{3}{2}} + 4n$,

2-28. *[5]* For each of the following expressions $f(n)$ find a simple $g(n)$ such that $f(n) = \Theta(g(n))$. (You should be able to prove your result by exhibiting the relevant parameters, but this is not required for the homework.)

(a) $f(n) = \sum_{i=1}^{n} 3i^4 + 2i^3 - 19i + 20$.

(b) $f(n) = \sum_{i=1}^{n} 3(4^i) + 2(3^i) - i^{19} + 20$.

(c) $f(n) = \sum_{i=1}^{n} 5^i + 3^{2i}$.

2-29. *[5]* Which of the following are true?

(a) $\sum_{i=1}^{n} 3^i = \Theta(3^{n-1})$.

(b) $\sum_{i=1}^{n} 3^i = \Theta(3^n)$.

(c) $\sum_{i=1}^{n} 3^i = \Theta(3^{n+1})$.

2-30. *[5]* For each of the following functions f find a simple function g such that $f(n) = \Theta(g(n))$.

(a) $f_1(n) = (1000)2^n + 4^n$.

(b) $f_2(n) = n + n\log n + \sqrt{n}$.

(c) $f_3(n) = \log(n^{20}) + (\log n)^{10}$.

(d) $f_4(n) = (0.99)^n + n^{100}$.

2-31. *[5]* For each pair of expressions (A, B) below, indicate whether A is O, o, Ω, ω, or Θ of B. Note that zero, one or more of these relations may hold for a given pair; list all correct ones.

	A	B
(a)	n^{100}	2^n
(b)	$(\lg n)^{12}$	$\sqrt{n}$
(c)	$\sqrt{n}$	$n^{\cos(\pi n/8)}$
(d)	10^n	100^n
(e)	$n^{\lg n}$	$(\lg n)^n$
(f)	$\lg(n!)$	$n \lg n$

Summations

2-32. *[5]* Prove that:

$$1^2 - 2^2 + 3^2 - 4^2 + \ldots + (-1)^{k-1}k^2 = (-1)^{k-1}k(k+1)/2$$

2-33. *[5]* Find an expression for the sum of the ith row of the following triangle, and prove its correctness. Each entry is the sum of the three entries directly above it. All non existing entries are considered 0.

				1				
			1	1	1			
		1	2	3	2	1		
	1	3	6	7	6	3	1	
1	4	10	16	19	16	10	4	1

2-34. *[3]* Assume that Christmas has n days. Exactly how many presents did my "true love" send me? (Do some research if you do not understand this question.)

2-35. *[5]* Consider the following code fragment.

```
for i=1 to n do
    for j=i to 2*i do
        output ‘‘foobar’’
```

Let $T(n)$ denote the number of times 'foobar' is printed as a function of n.

a. Express $T(n)$ as a summation (actually two nested summations).

b. Simplify the summation. Show your work.

2-36. *[5]* Consider the following code fragment.

```
for i=1 to n/2 do
    for j=i to n-i do
        for k=1 to j do
output ‘‘foobar’’
```

Assume n is even. Let $T(n)$ denote the number of times 'foobar' is printed as a function of n.

(a) Express $T(n)$ as three nested summations.

(b) Simplify the summation. Show your work.

2-37. *[6]* When you first learned to multiply numbers, you were told that $x \times y$ means adding x a total of y times, so $5 \times 4 = 5+5+5+5 = 20$. What is the time complexity of multiplying two n-digit numbers in base b (people work in base 10, of course, while computers work in base 2) using the repeated addition method, as a function of n and b. Assume that single-digit by single-digit addition or multiplication takes $O(1)$ time. (Hint: how big can y be as a function of n and b?)

2-38. *[6]* In grade school, you learned to multiply long numbers on a digit-by-digit basis, so that $127 \times 211 = 127 \times 1 + 127 \times 10 + 127 \times 200 = 26,397$. Analyze the time complexity of multiplying two n-digit numbers with this method as a function of n (assume constant base size). Assume that single-digit by single-digit addition or multiplication takes $O(1)$ time.

Logarithms

2-39. *[5]* Prove the following identities on logarithms:

(a) Prove that $\log_a(xy) = \log_a x + \log_a y$

(b) Prove that $\log_a x^y = y \log_a x$

(c) Prove that $\log_a x = \frac{\log_b x}{\log_b a}$

(d) Prove that $x^{\log_b y} = y^{\log_b x}$

2-40. *[3]* Show that $\lceil \lg(n+1) \rceil = \lfloor \lg n \rfloor + 1$

2-41. *[3]* Prove that that the binary representation of $n \geq 1$ has $\lfloor \lg_2 n \rfloor + 1$ bits.

2-42. *[5]* In one of my research papers I give a comparison-based sorting algorithm that runs in $O(n \log(\sqrt{n}))$. Given the existence of an $\Omega(n \log n)$ lower bound for sorting, how can this be possible?

Interview Problems

2-43. *[5]* You are given a set S of n numbers. You must pick a subset S' of k numbers from S such that the probability of each element of S occurring in S' is equal (i.e., each is selected with probability k/n). You may make only one pass over the numbers. What if n is unknown?

2-44. *[5]* We have 1,000 data items to store on 1,000 nodes. Each node can store copies of exactly three different items. Propose a replication scheme to minimize data loss as nodes fail. What is the expected number of data entries that get lost when three random nodes fail?

2-45. *[5]* Consider the following algorithm to find the minimum element in an array of numbers $A[0, \ldots, n]$. One extra variable *tmp* is allocated to hold the current minimum value. Start from A[0]; "tmp" is compared against $A[1]$, $A[2]$, $\ldots$, $A[N]$ in order. When $A[i] < tmp$, $tmp = A[i]$. What is the expected number of times that the assignment operation $tmp = A[i]$ is performed?

2-46. *[5]* You have a 100-story building and a couple of marbles. You must identify the lowest floor for which a marble will break if you drop it from this floor. How fast can you find this floor if you are given an infinite supply of marbles? What if you have only two marbles?

2-47. *[5]* You are given 10 bags of gold coins. Nine bags contain coins that each weigh 10 grams. One bag contains all false coins that weigh one gram less. You must identify this bag in just one weighing. You have a digital balance that reports the weight of what is placed on it.

2-48. *[5]* You have eight balls all of the same size. Seven of them weigh the same, and one of them weighs slightly more. How can you find the ball that is heavier by using a balance and only two weighings?

2-49. *[5]* Suppose we start with n companies that eventually merge into one big company. How many different ways are there for them to merge?

2-50. *[5]* A *Ramanujam number* can be written two different ways as the sum of two cubes—i.e. , there exist distinct a, b, c, and d such that $a^3 + b^3 = c^3 + d^3$. Generate all Ramanujam numbers where $a, b, c, d < n$.

2-51. *[7]* Six pirates must divide $300 dollars among themselves. The division is to proceed as follows. The senior pirate proposes a way to divide the money. Then the pirates vote. If the senior pirate gets at least half the votes he wins, and that division remains. If he doesn't, he is killed and then the next senior-most pirate gets a chance to do the division. Now you have to tell what will happen and why (i.e. , how many pirates survive and how the division is done)? All the pirates are intelligent and the first priority is to stay alive and the next priority is to get as much money as possible.

2-52. *[7]* Reconsider the pirate problem above, where only one indivisible dollar is to be divided. Who gets the dollar and how many are killed?

Programming Challenges

These programming challenge problems with robot judging are available at *http://www.programming-challenges.com* or *http://online-judge.uva.es*.

2-1. "Primary Arithmetic" – Programming Challenges 110501, UVA Judge 10035.

2-2. "A Multiplication Game" – Programming Challenges 110505, UVA Judge 847.

2-3. "Light, More Light" – Programming Challenges 110701, UVA Judge 10110.

3

Data Structures

Changing a data structure in a slow program can work the same way an organ transplant does in a sick patient. Important classes of *abstract data types* such as containers, dictionaries, and priority queues, have many different but functionally equivalent *data structures* that implement them. Changing the data structure does not change the correctness of the program, since we presumably replace a correct implementation with a different correct implementation. However, the new implementation of the data type realizes different tradeoffs in the time to execute various operations, so the total performance can improve dramatically. Like a patient in need of a transplant, only one part might need to be replaced in order to fix the problem.

But it is better to be born with a good heart than have to wait for a replacement. The maximum benefit from good data structures results from designing your program around them in the first place. We assume that the reader has had some previous exposure to elementary data structures and pointer manipulation. Still, data structure (CS II) courses these days focus more on data abstraction and object orientation than the nitty-gritty of how structures should be represented in memory. We will review this material to make sure you have it down.

In data structures, as with most subjects, it is more important to really understand the basic material than have exposure to more advanced concepts. We will focus on each of the three fundamental abstract data types (containers, dictionaries, and priority queues) and see how they can be implemented with arrays and lists. Detailed discussion of the tradeoffs between more sophisticated implementations is deferred to the relevant catalog entry for each of these data types.

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3.1 Contiguous vs. Linked Data Structures

Data structures can be neatly classified as either *contiguous* or *linked*, depending upon whether they are based on arrays or pointers:

- *Contiguously-allocated structures* are composed of single slabs of memory, and include arrays, matrices, heaps, and hash tables.
- *Linked data structures* are composed of distinct chunks of memory bound together by *pointers*, and include lists, trees, and graph adjacency lists.

In this section, we review the relative advantages of contiguous and linked data structures. These tradeoffs are more subtle than they appear at first glance, so I encourage readers to stick with me here even if you may be familiar with both types of structures.

3.1.1 Arrays

The *array* is the fundamental contiguously-allocated data structure. Arrays are structures of fixed-size data records such that each element can be efficiently located by its *index* or (equivalently) address.

A good analogy likens an array to a street full of houses, where each array element is equivalent to a house, and the index is equivalent to the house number. Assuming all the houses are equal size and numbered sequentially from 1 to n, we can compute the exact position of each house immediately from its address.[1]

Advantages of contiguously-allocated arrays include:

- *Constant-time access given the index* – Because the index of each element maps directly to a particular memory address, we can access arbitrary data items instantly provided we know the index.
- *Space efficiency* – Arrays consist purely of data, so no space is wasted with links or other formatting information. Further, end-of-record information is not needed because arrays are built from fixed-size records.
- *Memory locality* – A common programming idiom involves iterating through all the elements of a data structure. Arrays are good for this because they exhibit excellent memory locality. Physical continuity between successive data accesses helps exploit the high-speed *cache memory* on modern computer architectures.

The downside of arrays is that we cannot adjust their size in the middle of a program's execution. Our program will fail soon as we try to add the $(n +$

[1] Houses in Japanese cities are traditionally numbered in the order they were built, not by their physical location. This makes it extremely difficult to locate a Japanese address without a detailed map.

1)st customer, if we only allocate room for n records. We can compensate by allocating extremely large arrays, but this can waste space, again restricting what our programs can do.

Actually, we *can* efficiently enlarge arrays as we need them, through the miracle of *dynamic arrays*. Suppose we start with an array of size 1, and double its size from m to $2m$ each time we run out of space. This doubling process involves allocating a new contiguous array of size $2m$, copying the contents of the old array to the lower half of the new one, and returning the space used by the old array to the storage allocation system.

The apparent waste in this procedure involves the recopying of the old contents on each expansion. How many times might an element have to be recopied after a total of n insertions? Well, the first inserted element will have been recopied when the array expands after the first, second, fourth, eighth, ... insertions. It will take $\log_2 n$ doublings until the array gets to have n positions. However, most elements do not suffer much upheaval. Indeed, the $(n/2+1)$st through nth elements will move at most once and might never have to move at all.

If half the elements move once, a quarter of the elements twice, and so on, the total number of movements M is given by

$$M = \sum_{i=1}^{\lg n} i \cdot n/2^i = n \sum_{i=1}^{\lg n} i/2^i \leq n \sum_{i=1}^{\infty} i/2^i = 2n$$

Thus, each of the n elements move only two times on average, and the total work of managing the dynamic array is the same $O(n)$ as it would have been if a single array of sufficient size had been allocated in advance!

The primary thing lost using dynamic arrays is the guarantee that each array access takes constant time *in the worst case*. Now all the queries will be fast, except for those relatively few queries triggering array doubling. What we get instead is a promise that the nth array access will be completed quickly enough that the *total* effort expended so far will still be $O(n)$. Such *amortized* guarantees arise frequently in the analysis of data structures.

3.1.2 Pointers and Linked Structures

Pointers are the connections that hold the pieces of linked structures together. Pointers represent the address of a location in memory. A variable storing a pointer to a given data item can provide more freedom than storing a copy of the item itself. A cell-phone number can be thought of as a pointer to its owner as they move about the planet.

Pointer syntax and power differ significantly across programming languages, so we begin with a quick review of pointers in C language. A pointer `p` is assumed to

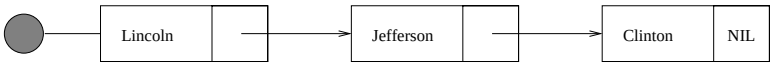

Figure 3.1: Linked list example showing data and pointer fields

give the address in memory where a particular chunk of data is located.[2] Pointers in C have types declared at compiler time, denoting the data type of the items they can point to. We use `*p` to denote the item that is pointed to by pointer `p`, and `&x` to denote the address (i.e. , pointer) of a particular variable `x`. A special `NULL` pointer value is used to denote structure-terminating or unassigned pointers.

All linked data structures share certain properties, as revealed by the following linked list type declaration:

```
typedef struct list {
        item_type item;                 /* data item */
        struct list *next;              /* point to successor */
} list;
```

In particular:

- Each node in our data structure (here `list`) contains one or more data fields (here `item`) that retain the data that we need to store.
- Each node contains a pointer field to at least one other node (here `next`). This means that much of the space used in linked data structures has to be devoted to pointers, not data.
- Finally, we need a pointer to the head of the structure, so we know where to access it.

The list is the simplest linked structure. The three basic operations supported by lists are searching, insertion, and deletion. In *doubly-linked lists*, each node points both to its predecessor and its successor element. This simplifies certain operations at a cost of an extra pointer field per node.

Searching a List

Searching for item x in a linked list can be done iteratively or recursively. We opt for recursively in the implementation below. If x is in the list, it is either the first element or located in the smaller rest of the list. Eventually, we reduce the problem to searching in an empty list, which clearly cannot contain x.

[2] C permits direct manipulation of memory addresses in ways which may horrify Java programmers, but we will avoid doing any such tricks.

```
list *search_list(list *l, item_type x)
{
        if (l == NULL) return(NULL);

        if (l->item == x)
                return(l);
        else
                return( search_list(l->next, x) );
}
```

Insertion into a List

Insertion into a singly-linked list is a nice exercise in pointer manipulation, as shown below. Since we have no need to maintain the list in any particular order, we might as well insert each new item in the simplest place. Insertion at the beginning of the list avoids any need to traverse the list, but does require us to update the pointer (denoted `l`) to the head of the data structure.

```
void insert_list(list **l, item_type x)
{
        list *p;                        /* temporary pointer */

        p = malloc( sizeof(list) );
        p->item = x;
        p->next = *l;
        *l = p;
}
```

Two C-isms to note. First, the `malloc` function allocates a chunk of memory of sufficient size for a new node to contain `x`. Second, the funny double star (`**l`) denotes that `l` is a *pointer to a pointer* to a list node. Thus the last line, `*l=p;` copies `p` to the place pointed to `l`, which is the external variable maintaining access to the head of the list.

Deletion From a List

Deletion from a linked list is somewhat more complicated. First, we must find a pointer to the *predecessor* of the item to be deleted. We do this recursively:

```
list *predecessor_list(list *l, item_type x)
{
        if ((l == NULL) || (l->next == NULL)) {
                printf("Error: predecessor sought on null list.\n");
                return(NULL);
        }

        if ((l->next)->item == x)
                return(l);
        else
                return( predecessor_list(l->next, x) );
}
```

The predecessor is needed because it points to the doomed node, so its `next` pointer must be changed. The actual deletion operation is simple, once ruling out the case that the to-be-deleted element does not exist. Special care must be taken to reset the pointer to the head of the list (`l`) when the first element is deleted:

```
delete_list(list **l, item_type x)
{
        list *p;                        /* item pointer */
        list *pred;                     /* predecessor pointer */
        list *search_list(), *predecessor_list();

        p = search_list(*l,x);
        if (p != NULL) {
                pred = predecessor_list(*l,x);
                if (pred == NULL)       /* splice out out list */
                        *l = p->next;
                else
                        pred->next = p->next;

                free(p);                /* free memory used by node */
        }
}
```

C language requires explicit deallocation of memory, so we must `free` the deleted node after we are finished with it to return the memory to the system.

3.1.3 Comparison

The relative advantages of linked lists over static arrays include:

- Overflow on linked structures can never occur unless the memory is actually full.

- Insertions and deletions are *simpler* than for contiguous (array) lists.
- With large records, moving pointers is easier and faster than moving the items themselves.

while the relative advantages of arrays include:

- Linked structures require extra space for storing pointer fields.
- Linked lists do not allow efficient random access to items.
- Arrays allow better memory locality and cache performance than random pointer jumping.

Take-Home Lesson: Dynamic memory allocation provides us with flexibility on how and where we use our limited storage resources.

One final thought about these fundamental structures is that they can be thought of as recursive objects:

- *Lists* – Chopping the first element off a linked list leaves a smaller linked list. This same argument works for strings, since removing characters from string leaves a string. Lists are recursive objects.
- *Arrays* – Splitting the first k elements off of an n element array gives two smaller arrays, of size k and $n-k$, respectively. Arrays are recursive objects.

This insight leads to simpler list processing, and efficient divide-and-conquer algorithms such as quicksort and binary search.

3.2 Stacks and Queues

We use the term *container* to denote a data structure that permits storage and retrieval of data items *independent of content*. By contrast, dictionaries are abstract data types that retrieve based on key values or content, and will be discussed in Section 3.3 (page 72).

Containers are distinguished by the particular retrieval order they support. In the two most important types of containers, this retrieval order depends on the insertion order:

- *Stacks* – Support retrieval by last-in, first-out (LIFO) order. Stacks are simple to implement and very efficient. For this reason, stacks are probably the right container to use when retrieval order doesn't matter at all, such as when processing batch jobs. The *put* and *get* operations for stacks are usually called *push* and *pop*:

  - *Push(x,s)*: Insert item x at the top of stack s.
  - *Pop(s)*: Return (and remove) the top item of stack s.

  LIFO order arises in many real-world contexts. People crammed into a subway car exit in LIFO order. Food inserted into my refrigerator usually exits the same way, despite the incentive of expiration dates. Algorithmically, LIFO tends to happen in the course of executing recursive algorithms.

- *Queues* – Support retrieval in first in, first out (FIFO) order. This is surely the fairest way to control waiting times for services. You want the container holding jobs to be processed in FIFO order to minimize the *maximum* time spent waiting. Note that the *average* waiting time will be the same regardless of whether FIFO or LIFO is used. Many computing applications involve data items with infinite patience, which renders the question of maximum waiting time moot.

  Queues are somewhat trickier to implement than stacks and thus are most appropriate for applications (like certain simulations) where the order is important. The *put* and *get* operations for queues are usually called *enqueue* and *dequeue*.

  - *Enqueue(x,q)*: Insert item x at the back of queue q.
  - *Dequeue(q)*: Return (and remove) the front item from queue q.

  We will see queues later as the fundamental data structure controlling breadth-first searches in graphs.

Stacks and queues can be effectively implemented using either arrays or linked lists. The key issue is whether an upper bound on the size of the container is known in advance, thus permitting the use of a statically-allocated array.

3.3 Dictionaries

The *dictionary* data type permits access to data items by content. You stick an item into a dictionary so you can find it when you need it.

The primary operations of dictionary support are:

- *Search(D,k)* – Given a search key k, return a pointer to the element in dictionary D whose key value is k, if one exists.
- *Insert(D,x)* – Given a data item x, add it to the set in the dictionary D.
- *Delete(D,x)* – Given a pointer to a given data item x in the dictionary D, remove it from D.

Certain dictionary data structures also efficiently support other useful operations:

- *Max(D)* or *Min(D)* – Retrieve the item with the largest (or smallest) key from D. This enables the dictionary to serve as a priority queue, to be discussed in Section 3.5 (page 83).
- *Predecessor(D,k)* or *Successor(D,k)* – Retrieve the item from D whose key is immediately before (or after) k in sorted order. These enable us to iterate through the elements of the data structure.

Many common data processing tasks can be handled using these dictionary operations. For example, suppose we want to remove all duplicate names from a mailing list, and print the results in sorted order. Initialize an empty dictionary D, whose search key will be the record name. Now read through the mailing list, and for each record *search* to see if the name is already in D. If not, *insert* it into D. Once finished, we must extract the remaining names out of the dictionary. By starting from the first item *Min(D)* and repeatedly calling *Successor* until we obtain *Max(D)*, we traverse all elements in sorted order.

By defining such problems in terms of abstract dictionary operations, we avoid the details of the data structure's representation and focus on the task at hand.

In the rest of this section, we will carefully investigate simple dictionary implementations based on arrays and linked lists. More powerful dictionary implementations such as binary search trees (see Section 3.4 (page 77)) and hash tables (see Section 3.7 (page 89)) are also attractive options in practice. A complete discussion of different dictionary data structures is presented in the catalog in Section 12.1 (page 367). We encourage the reader to browse through the data structures section of the catalog to better learn what your options are.

Stop and Think: Comparing Dictionary Implementations (I)

Problem: What are the asymptotic worst-case running times for each of the seven fundamental dictionary operations (search, insert, delete, successor, predecessor, minimum, and maximum) when the data structure is implemented as:

- An unsorted array.
- A sorted array.

Solution: This problem (and the one following it) reveal some of the inherent tradeoffs of data structure design. A given data representation may permit efficient implementation of certain operations at the cost that other operations are expensive.

In addition to the array in question, we will assume access to a few extra variables such as n—the number of elements currently in the array. Note that we must *maintain* the value of these variables in the operations where they change (e.g., insert and delete), and charge these operations the cost of this maintenance.

The basic dictionary operations can be implemented with the following costs on unsorted and sorted arrays, respectively:

Dictionary operation	Unsorted array	Sorted array
Search(L, k)	$O(n)$	$O(\log n)$
Insert(L, x)	$O(1)$	$O(n)$
Delete(L, x)	$O(1)^*$	$O(n)$
Successor(L, x)	$O(n)$	$O(1)$
Predecessor(L, x)	$O(n)$	$O(1)$
Minimum(L)	$O(n)$	$O(1)$
Maximum(L)	$O(n)$	$O(1)$

We must understand the implementation of each operation to see why. First, we discuss the operations when maintaining an *unsorted* array A.

- *Search* is implemented by testing the search key k against (potentially) each element of an unsorted array. Thus, search takes linear time in the worst case, which is when key k is not found in A.
- *Insertion* is implemented by incrementing n and then copying item x to the nth cell in the array, $A[n]$. The bulk of the array is untouched, so this operation takes constant time.
- *Deletion* is somewhat trickier, hence the superscript(*) in the table. The definition states that we are given a pointer x to the element to delete, so we need not spend any time searching for the element. But removing the xth element from the array A leaves a hole that must be filled. We could fill the hole by moving each of the elements $A[x+1]$ to $A[n]$ up one position, but this requires $\Theta(n)$ time when the first element is deleted. The following idea is better: just write over $A[x]$ with $A[n]$, and decrement n. This only takes constant time.
- The definition of the traversal operations, *Predecessor* and *Successor*, refer to the item appearing before/after x *in sorted order*. Thus, the answer is not simply $A[x-1]$ (or $A[x+1]$), because in an unsorted array an element's physical predecessor (successor) is not necessarily its logical predecessor (successor). Instead, the predecessor of $A[x]$ is the biggest element smaller than $A[x]$. Similarly, the successor of $A[x]$ is the smallest element larger than $A[x]$. Both require a sweep through all n elements of A to determine the winner.
- *Minimum* and *Maximum* are similarly defined with respect to sorted order, and so require linear sweeps to identify in an unsorted array.

Implementing a dictionary using a *sorted* array completely reverses our notions of what is easy and what is hard. Searches can now be done in $O(\log n)$ time, using binary search, because we know the median element sits in $A[n/2]$. Since the upper and lower portions of the array are also sorted, the search can continue recursively on the appropriate portion. The number of halvings of n until we get to a single element is $\lceil \lg n \rceil$.

The sorted order also benefits us with respect to the other dictionary retrieval operations. The minimum and maximum elements sit in $A[1]$ and $A[n]$, while the predecessor and successor to $A[x]$ are $A[x-1]$ and $A[x+1]$, respectively.

Insertion and deletion become more expensive, however, because making room for a new item or filling a hole may require moving many items arbitrarily. Thus both become linear-time operations. ∎

> *Take-Home Lesson:* Data structure design must balance all the different operations it supports. The fastest data structure to support both operations A and B may well not be the fastest structure to support either operation A or B.

Stop and Think: Comparing Dictionary Implementations (II)

Problem: What is the asymptotic worst-case running times for each of the seven fundamental dictionary operations when the data structure is implemented as

- A singly-linked unsorted list.
- A doubly-linked unsorted list.
- A singly-linked sorted list.
- A doubly-linked sorted list.

Solution: Two different issues must be considered in evaluating these implementations: singly- vs. doubly-linked lists and sorted vs. unsorted order. Subtle operations are denoted with a superscript:

Dictionary operation	Singly unsorted	Double unsorted	Singly sorted	Doubly sorted
Search(L, k)	$O(n)$	$O(n)$	$O(n)$	$O(n)$
Insert(L, x)	$O(1)$	$O(1)$	$O(n)$	$O(n)$
Delete(L, x)	$O(n)^*$	$O(1)$	$O(n)^*$	$O(1)$
Successor(L, x)	$O(n)$	$O(n)$	$O(1)$	$O(1)$
Predecessor(L, x)	$O(n)$	$O(n)$	$O(n)^*$	$O(1)$
Minimum(L)	$O(n)$	$O(n)$	$O(1)$	$O(1)$
Maximum(L)	$O(n)$	$O(n)$	$O(1)^*$	$O(1)$

As with unsorted arrays, search operations are destined to be slow while maintenance operations are fast.

- *Insertion/Deletion* – The complication here is deletion from a singly-linked list. The definition of the *Delete* operation states we are given a pointer x to the item to be deleted. But what we *really* need is a pointer to the element pointing to x in the list, because that is the node that needs to be changed. We can do nothing without this list predecessor, and so must spend linear time searching for it on a singly-linked list. Doubly-linked lists avoid this problem, since we can immediately retrieve the list predecessor of x.

  Deletion is faster for sorted doubly-linked lists than sorted arrays, because splicing out the deleted element from the list is more efficient than filling the hole by moving array elements. The predecessor pointer problem again complicates deletion from singly-linked sorted lists.

- *Search* – Sorting provides less benefit for linked lists than it did for arrays. Binary search is no longer possible, because we can't access the median element without traversing all the elements before it. What sorted lists *do* provide is quick termination of unsuccessful searches, for if we have not found *Abbott* by the time we hit *Costello* we can deduce that he doesn't exist. Still, searching takes linear time in the worst case.

- *Traversal operations* – The predecessor pointer problem again complicates implementing *Predecessor*. The logical successor is equivalent to the node successor for both types of sorted lists, and hence can be implemented in constant time.

- *Maximum* – The maximum element sits at the tail of the list, which would normally require $\Theta(n)$ time to reach in either singly- or doubly-linked lists.

  However, we can maintain a separate pointer to the list tail, provided we pay the maintenance costs for this pointer on every insertion and deletion. The tail pointer can be updated in constant time on doubly-linked lists: on insertion check whether `last->next` still equals `NULL`, and on deletion set `last` to point to the list predecessor of `last` if the last element is deleted.

  We have no efficient way to find this predecessor for singly-linked lists. So why can we implement maximum in $\Theta(1)$ on singly-linked lists? The trick is to charge the cost to each deletion, which *already* took linear time. Adding an extra linear sweep to update the pointer does not harm the asymptotic complexity of *Delete*, while gaining us *Maximum* in constant time as a reward for clear thinking. ∎

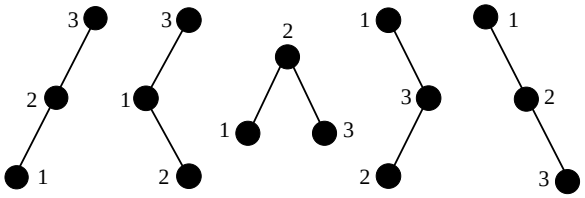

Figure 3.2: The five distinct binary search trees on three nodes

3.4 Binary Search Trees

We have seen data structures that allow fast search or flexible update, but not fast search *and* flexible update. Unsorted, doubly-linked lists supported insertion and deletion in $O(1)$ time but search took linear time in the worse case. Sorted arrays support binary search and logarithmic query times, but at the cost of linear-time update.

Binary search requires that we have fast access to *two elements*—specifically the median elements above and below the given node. To combine these ideas, we need a "linked list" with two pointers per node. This is the basic idea behind binary search trees.

A *rooted binary tree* is recursively defined as either being (1) empty, or (2) consisting of a node called the root, together with two rooted binary trees called the left and right subtrees, respectively. The order among "brother" nodes matters in rooted trees, so left is different from right. Figure 3.2 gives the shapes of the five distinct binary trees that can be formed on three nodes.

A binary *search* tree labels each node in a binary tree with a single key such that for any node labeled x, all nodes in the left subtree of x have keys $< x$ while all nodes in the right subtree of x have keys $> x$. This search tree labeling scheme is very special. For any binary tree on n nodes, and any set of n keys, there is *exactly* one labeling that makes it a binary search tree. The allowable labelings for three-node trees are given in Figure 3.2.

3.4.1 Implementing Binary Search Trees

Binary tree nodes have *left* and *right* pointer fields, an (optional) *parent* pointer, and a data field. These relationships are shown in Figure 3.3; a type declaration for the tree structure is given below:

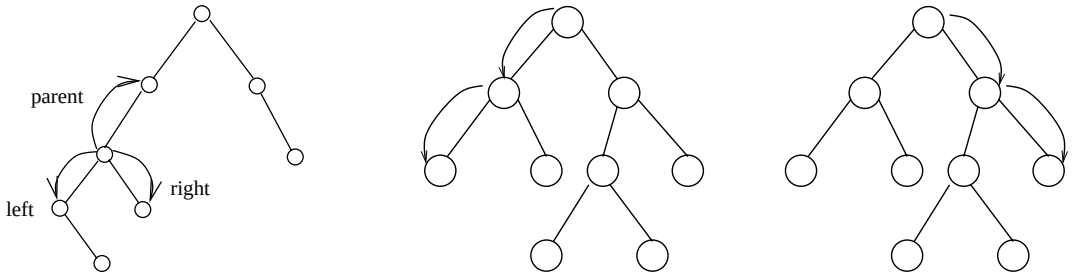

Figure 3.3: Relationships in a binary search tree (left). Finding the minimum (center) and maximum (right) elements in a binary search tree

```
typedef struct tree {
        item_type item;                 /* data item */
        struct tree *parent;            /* pointer to parent */
        struct tree *left;              /* pointer to left child */
        struct tree *right;             /* pointer to right child */
} tree;
```

The basic operations supported by binary trees are searching, traversal, insertion, and deletion.

Searching in a Tree

The binary search tree labeling uniquely identities where each key is located. Start at the root. Unless it contains the query key x, proceed either left or right depending upon whether x occurs before or after the root key. This algorithm works because both the left and right subtrees of a binary search tree are themselves binary search trees. This recursive structure yields the recursive search algorithm below:

```
tree *search_tree(tree *l, item_type x)
{
        if (l == NULL) return(NULL);

        if (l->item == x) return(l);

        if (x < l->item)
                return( search_tree(l->left, x) );
        else
                return( search_tree(l->right, x) );
}
```

This search algorithm runs in $O(h)$ time, where h denotes the height of the tree.

Finding Minimum and Maximum Elements in a Tree

Implementing the *find-minimum* operation requires knowing where the minimum element is in the tree. By definition, the smallest key must reside in the left subtree of the root, since all keys in the left subtree have values less than that of the root. Therefore, as shown in Figure 3.3, the minimum element must be the leftmost descendent of the root. Similarly, the maximum element must be the rightmost descendent of the root.

```
tree *find_minimum(tree *t)
{
        tree *min;                      /* pointer to minimum */

        if (t == NULL) return(NULL);

        min = t;
        while (min->left != NULL)
                min = min->left;
        return(min);
}
```

Traversal in a Tree

Visiting all the nodes in a rooted binary tree proves to be an important component of many algorithms. It is a special case of traversing all the nodes and edges in a graph, which will be the foundation of Chapter 5.

A prime application of tree traversal is listing the labels of the tree nodes. Binary search trees make it easy to report the labels in sorted order. By definition, all the keys smaller than the root must lie in the left subtree of the root, and all keys bigger than the root in the right subtree. Thus, visiting the nodes recursively in accord with such a policy produces an *in-order* traversal of the search tree:

```
void traverse_tree(tree *l)
{
        if (l != NULL) {
                traverse_tree(l->left);
                process_item(l->item);
                traverse_tree(l->right);
        }

}
```

Each item is processed once during the course of traversal, which runs in $O(n)$ time, where n denotes the number of nodes in the tree.

Alternate traversal orders come from changing the position of `process_item` relative to the traversals of the left and right subtrees. Processing the item first yields a *pre-order* traversal, while processing it last gives a *post-order* traversal. These make relatively little sense with search trees, but prove useful when the rooted tree represents arithmetic or logical expressions.

Insertion in a Tree

There is only one place to insert an item x into a binary search tree T where we know we can find it again. We must replace the `NULL` pointer found in T after an unsuccessful query for the key k.

This implementation uses recursion to combine the search and node insertion stages of key insertion. The three arguments to `insert_tree` are (1) a pointer `l` to the pointer linking the search subtree to the rest of the tree, (2) the key `x` to be inserted, and (3) a `parent` pointer to the parent node containing `l`. The node is allocated and linked in on hitting the `NULL` pointer. Note that we pass the *pointer* to the appropriate left/right pointer in the node during the search, so the assignment `*l = p;` links the new node into the tree:

```
insert_tree(tree **l, item_type x, tree *parent)
{
    tree *p;                          /* temporary pointer */

    if (*l == NULL) {
           p = malloc(sizeof(tree)); /* allocate new node */
           p->item = x;
           p->left = p->right = NULL;
           p->parent = parent;
           *l = p;                    /* link into parent's record */
           return;
    }

    if (x < (*l)->item)
           insert_tree(&((*l)->left), x, *l);
    else
           insert_tree(&((*l)->right), x, *l);
}
```

Allocating the node and linking it in to the tree is a constant-time operation after the search has been performed in $O(h)$ time.

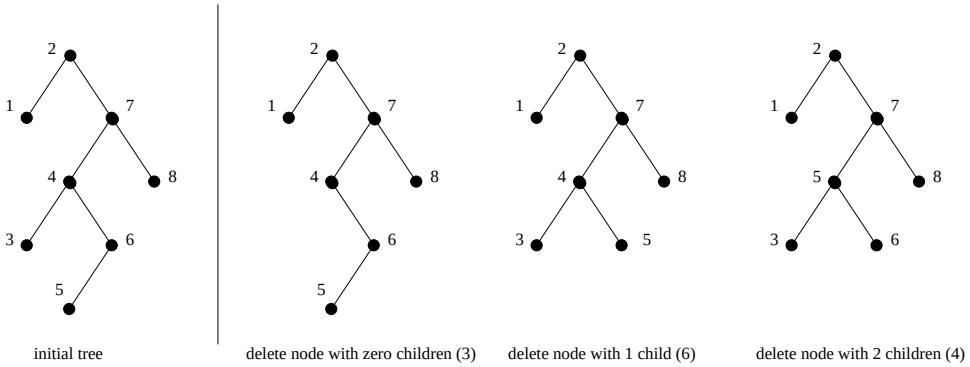

Figure 3.4: Deleting tree nodes with 0, 1, and 2 children

Deletion from a Tree

Deletion is somewhat trickier than insertion, because removing a node means appropriately linking its two descendant subtrees back into the tree somewhere else. There are three cases, illustrated in Figure 3.4. Leaf nodes have no children, and so may be deleted by simply clearing the pointer to the given node.

The case of the doomed node having one child is also straightforward. There is one parent and one grandchild, and we can link the grandchild directly to the parent without violating the in-order labeling property of the tree.

But what of a to-be-deleted node with two children? Our solution is to relabel this node with the key of its immediate successor in sorted order. This successor must be the smallest value in the right subtree, specifically the leftmost descendant in the right subtree (`p`). Moving this to the point of deletion results in a properly-labeled binary search tree, and reduces our deletion problem to physically removing a node with at most one child—a case that has been resolved above.

The full implementation has been omitted here because it looks a little ghastly, but the code follows logically from the description above.

The worst-case complexity analysis is as follows. Every deletion requires the cost of at most two search operations, each taking $O(h)$ time where h is the height of the tree, plus a constant amount of pointer manipulation.

3.4.2 How Good Are Binary Search Trees?

When implemented using binary search trees, all three dictionary operations take $O(h)$ time, where h is the height of the tree. The smallest height we can hope for occurs when the tree is perfectly balanced, where $h = \lceil \log n \rceil$. This is very good, but the tree must be perfectly balanced.

Our insertion algorithm puts each new item at a leaf node where it should have been found. This makes the shape (and more importantly height) of the tree a function of the order in which we insert the keys.

Unfortunately, bad things can happen when building trees through insertion. The data structure has no control over the order of insertion. Consider what happens if the user inserts the keys in sorted order. The operations `insert(`a`)`, followed by `insert(`b`)`, `insert(`c`)`, `insert(`d`)`, ... will produce a skinny linear height tree where only right pointers are used.

Thus binary trees can have heights ranging from $\lg n$ to n. But how tall are they on average? The average case analysis of algorithms can be tricky because we must carefully specify what we mean by *average*. The question is well defined if we consider each of the $n!$ possible insertion orderings equally likely and average over those. If so, we are in luck, because with high probability the resulting tree will have $O(\log n)$ height. This will be shown in Section 4.6 (page 123).

This argument is an important example of the power of *randomization*. We can often develop simple algorithms that offer good performance with high probability. We will see that a similar idea underlies the fastest known sorting algorithm, quicksort.

3.4.3 Balanced Search Trees

Random search trees are *usually* good. But if we get unlucky with our order of insertion, we can end up with a linear-height tree in the worst case. This worst case is outside of our direct control, since we must build the tree in response to the requests given by our potentially nasty user.

What would be better is an insertion/deletion procedure which *adjusts* the tree a little after each insertion, keeping it close enough to be balanced so the maximum height is logarithmic. Sophisticated *balanced* binary search tree data structures have been developed that guarantee the height of the tree always to be $O(\log n)$. Therefore, all dictionary operations (insert, delete, query) take $O(\log n)$ time each. Implementations of balanced tree data structures such as red-black trees and splay trees are discussed in Section 12.1 (page 367).

From an algorithm design viewpoint, it is important to know that these trees exist and that they can be used as black boxes to provide an efficient dictionary implementation. When figuring the costs of dictionary operations for algorithm analysis, we can assume the worst-case complexities of balanced binary trees to be a fair measure.

> *Take-Home Lesson:* Picking the wrong data structure for the job can be disastrous in terms of performance. Identifying the very best data structure is usually not as critical, because there can be several choices that perform similarly.

Stop and Think: Exploiting Balanced Search Trees

Problem: You are given the task of reading n numbers and then printing them out in sorted order. Suppose you have access to a balanced dictionary data structure, which supports the operations search, insert, delete, minimum, maximum, successor, and predecessor each in $O(\log n)$ time.

1. How can you sort in $O(n \log n)$ time using only insert and in-order traversal?
2. How can you sort in $O(n \log n)$ time using only minimum, successor, and insert?
3. How can you sort in $O(n \log n)$ time using only minimum, insert, delete, search?

Solution: The first problem allows us to do insertion and inorder-traversal. We can build a search tree by inserting all n elements, then do a traversal to access the items in sorted order:

```
Sort1()
    initialize-tree(t)
    While (not EOF)
        read(x);
        insert(x,t)
    Traverse(t)
```

```
Sort2()
    initialize-tree(t)
    While (not EOF)
        read(x);
        insert(x,t);
    y = Minimum(t)
    While (y ≠ NULL) do
        print(y → item)
        y = Successor(y,t)
```

```
Sort3()
    initialize-tree(t)
    While (not EOF)
        read(x);
        insert(x,t);
    y = Minimum(t)
    While (y ≠ NULL) do
        print(y→item)
        Delete(y,t)
        y = Minimum(t)
```

The second problem allows us to use the minimum and successor operations after constructing the tree. We can start from the minimum element, and then repeatedly find the successor to traverse the elements in sorted order.

The third problem does not give us successor, but does allow us delete. We can repeatedly find and delete the minimum element to once again traverse all the elements in sorted order.

Each of these algorithms does a linear number of logarithmic-time operations, and hence runs in $O(n \log n)$ time. The key to exploiting balanced binary search trees is using them as black boxes. ∎

3.5 Priority Queues

Many algorithms process items in a specific order. For example, suppose you must schedule jobs according to their importance relative to other jobs. Scheduling the

jobs requires sorting them by importance, and then evaluating them in this sorted order.

Priority queues are data structures that provide more flexibility than simple sorting, because they allow new elements to enter a system at arbitrary intervals. It is much more cost-effective to insert a new job into a priority queue than to re-sort everything on each such arrival.

The basic priority queue supports three primary operations:

- *Insert(Q,x)*– Given an item x with key k, insert it into the priority queue Q.
- *Find-Minimum(Q)* or *Find-Maximum(Q)*– Return a pointer to the item whose key value is smaller (larger) than any other key in the priority queue Q.
- *Delete-Minimum(Q)* or *Delete-Maximum(Q)*– Remove the item from the priority queue Q whose key is minimum (maximum).

Many naturally occurring processes are accurately modeled by priority queues. Single people maintain a priority queue of potential dating candidates—mentally if not explicitly. One's impression on meeting a new person maps directly to an attractiveness or desirability score. Desirability serves as the *key* field for inserting this new entry into the "little black book" priority queue data structure. Dating is the process of extracting the most desirable person from the data structure (Find-Maximum), spending an evening to evaluate them better, and then reinserting them into the priority queue with a possibly revised score.

Take-Home Lesson: Building algorithms around data structures such as dictionaries and priority queues leads to both clean structure and good performance.

Stop and Think: Basic Priority Queue Implementations

Problem: What is the worst-case time complexity of the three basic priority queue operations (insert, find-minimum, and delete-minimum) when the basic data structure is

- An unsorted array.
- A sorted array.
- A balanced binary search tree.

Solution: There is surprising subtlety in implementing these three operations, even when using a data structure as simple as an unsorted array. The unsorted array

dictionary (discussed on page 73) implemented insertion and deletion in constant time, and search and minimum in linear time. A linear time implementation of delete-minimum can be composed from *find-minimum*, followed by *search*, followed by *delete*.

For sorted arrays, we can implement insert and delete in linear time, and minimum in constant time. However, all priority queue deletions involve only the minimum element. By storing the sorted array in reverse order (largest value on top), the minimum element will be the last one in the array. Deleting the tail element requires no movement of any items, just decrementing the number of remaining items n, and so delete-minimum can be implemented in constant time.

All this is fine, yet the following table claims we can implement find-minimum in constant time for each data structure:

	Unsorted array	Sorted array	Balanced tree
Insert(Q, x)	$O(1)$	$O(n)$	$O(\log n)$
Find-Minimum(Q)	$O(1)$	$O(1)$	$O(1)$
Delete-Minimum(Q)	$O(n)$	$O(1)$	$O(\log n)$

The trick is using an extra variable to store a pointer/index to the minimum entry in each of these structures, so we can simply return this value whenever we are asked to find-minimum. Updating this pointer on each insertion is easy—we update it if and only if the newly inserted value is less than the current minimum. But what happens on a delete-minimum? We can delete the minimum entry *have*, then do an honest find-minimum to restore our canned value. The honest find-minimum takes linear time on an unsorted array and logarithmic time on a tree, and hence can be folded into the cost of each deletion. ∎

Priority queues are very useful data structures. Indeed, they will be the hero of two of our war stories, including the next one. A particularly nice priority queue implementation (the heap) will be discussed in the context of sorting in Section 4.3 (page 108). Further, a complete set of priority queue implementations is presented in Section 12.2 (page 373) of the catalog.

3.6 War Story: Stripping Triangulations

Geometric models used in computer graphics are commonly represented as a triangulated surface, as shown in Figure 3.5(l). High-performance rendering engines have special hardware for rendering and shading triangles. This hardware is so fast that the bottleneck of rendering is the cost of feeding the triangulation structure into the hardware engine.

Although each triangle can be described by specifying its three endpoints, an alternative representation is more efficient. Instead of specifying each triangle in isolation, suppose that we partition the triangles into *strips* of adjacent triangles

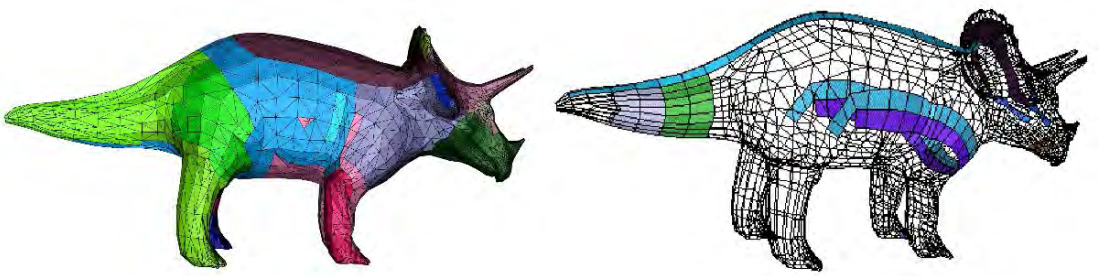

Figure 3.5: (l) A triangulated model of a dinosaur (r) Several triangle strips in the model

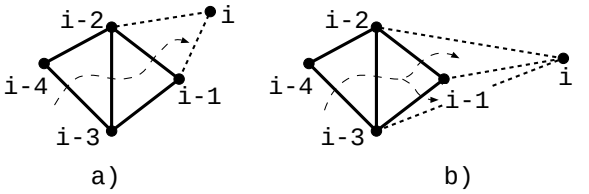

Figure 3.6: Partitioning a triangular mesh into strips: (a) with left-right turns (b) with the flexibility of arbitrary turns

and walk along the strip. Since each triangle shares two vertices in common with its neighbors, we save the cost of retransmitting the two extra vertices and any associated information. To make the description of the triangles unambiguous, the *OpenGL* triangular-mesh renderer assumes that all turns alternate from left to right (as shown in Figure 3.6).

The task of finding a small number of strips that cover each triangle in a mesh can be thought of as a graph problem. The graph of interest has a vertex for every *triangle* of the mesh, and an edge between every pair of vertices representing adjacent triangles. This *dual graph* representation captures all the information about the triangulation (see Section 15.12 (page 520)) needed to partition it into triangular strips.

Once we had the dual graph available, the project could begin in earnest. We sought to partition the vertices into as few paths or strips as possible. Partitioning it into one path implied that we had discovered a Hamiltonian path, which by definition visits each vertex exactly once. Since finding a Hamiltonian path is NP-complete (see Section 16.5 (page 538)), we knew not to look for an optimal algorithm, but concentrate instead on heuristics.

The simplest heuristic for strip cover would start from an arbitrary triangle and then do a left-right walk until the walk ends, either by hitting the boundary of

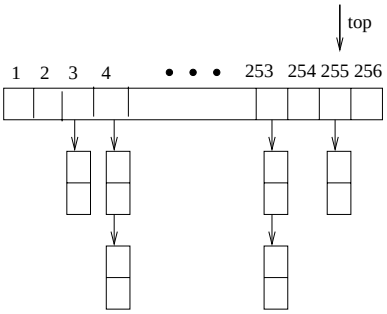

Figure 3.7: A bounded height priority queue for triangle strips

the object or a previously visited triangle. This heuristic had the advantage that it would be fast and simple, although there is no reason why it should find the smallest possible set of left-right strips for a given triangulation.

The *greedy* heuristic would be more likely to result in a small number of strips however. Greedy heuristics always try to grab the best possible thing first. In the case of the triangulation, the natural greedy heuristic would identify the starting triangle that yields the longest left-right strip, and peel that one off first.

Being greedy does not guarantee you the best possible solution either, since the first strip you peel off might break apart a lot of potential strips we might have wanted to use later. Still, being greedy is a good rule of thumb if you want to get rich. Since removing the longest strip would leave the fewest number of triangles for later strips, the greedy heuristic should outperform the naive heuristic.

But how much time does it take to find the largest strip to peel off next? Let k be the length of the walk possible from an average vertex. Using the simplest possible implementation, we could walk from each of the n vertices to find the largest remaining strip to report in $O(kn)$ time. Repeating this for each of the roughly n/k strips we extract yields an $O(n^2)$-time implementation, which would be hopelessly slow on a typical model of 20,000 triangles.

How could we speed this up? It seems wasteful to rewalk from each triangle after deleting a single strip. We could maintain the lengths of all the possible future strips in a data structure. However, whenever we peel off a strip, we must update the lengths of all affected strips. These strips will be shortened because they walked through a triangle that now no longer exists. There are two aspects of such a data structure:

- *Priority Queue* – Since we were repeatedly identifying the longest remaining strip, we needed a priority queue to store the strips ordered according to length. The next strip to peel always sat at the top of the queue. Our priority queue had to permit reducing the priority of arbitrary elements of the queue whenever we updated the strip lengths to reflect what triangles were peeled

Model name	Triangle count	Naive cost	Greedy cost	Greedy time
Diver	3,798	8,460	4,650	6.4 sec
Heads	4,157	10,588	4,749	9.9 sec
Framework	5,602	9,274	7,210	9.7 sec
Bart Simpson	9,654	24,934	11,676	20.5 sec
Enterprise	12,710	29,016	13,738	26.2 sec
Torus	20,000	40,000	20,200	272.7 sec
Jaw	75,842	104,203	95,020	136.2 sec

Figure 3.8: A comparison of the naive versus greedy heuristics for several triangular meshes

away. Because all of the strip lengths were bounded by a fairly small integer (hardware constraints prevent any strip from having more than 256 vertices), we used a bounded-height priority queue (an array of buckets shown in Figure 3.7 and described in Section 12.2 (page 373)). An ordinary heap would also have worked just fine.

To update the queue entry associated with each triangle, we needed to quickly find where it was. This meant that we also needed a ...

- *Dictionary* – For each triangle in the mesh, we needed to find where it was in the queue. This meant storing a pointer to each triangle in a dictionary. By integrating this dictionary with the priority queue, we built a data structure capable of a wide range of operations.

Although there were various other complications, such as quickly recalculating the length of the strips affected by the peeling, the key idea needed to obtain better performance was to use the priority queue. Run time improved by several orders of magnitude after employing this data structure.

How much better did the greedy heuristic do than the naive heuristic? Consider the table in Figure 3.8. In all cases, the greedy heuristic led to a set of strips that cost less, as measured by the total size of the strips. The savings ranged from about 10% to 50%, which is quite remarkable since the greatest possible improvement (going from three vertices per triangle down to one) yields a savings of only 66.6%.

After implementing the greedy heuristic with our priority queue data structure, the program ran in $O(n \cdot k)$ time, where n is the number of triangles and k is the length of the average strip. Thus the torus, which consisted of a small number of very long strips, took longer than the jaw, even though the latter contained over three times as many triangles.

There are several lessons to be gleaned from this story. First, when working with a large enough data set, only linear or near linear algorithms (say $O(n \log n)$) are likely to be fast enough. Second, choosing the right data structure is often the key to getting the time complexity down to this point. Finally, using smart heuristic

like greedy is likely to significantly improve quality over the naive approach. How much the improvement will be can only be determined by experimentation.

3.7 Hashing and Strings

Hash tables are a *very* practical way to maintain a dictionary. They exploit the fact that looking an item up in an array takes constant time once you have its index. A hash function is a mathematical function that maps keys to integers. We will use the value of our hash function as an index into an array, and store our item at that position.

The first step of the hash function is usually to map each key to a big integer. Let α be the size of the alphabet on which a given string S is written. Let `char(c)` be a function that maps each symbol of the alphabet to a unique integer from 0 to $\alpha - 1$. The function

$$H(S) = \sum_{i=0}^{|S|-1} \alpha^{|S|-(i+1)} \times char(s_i)$$

maps each string to a unique (but large) integer by treating the characters of the string as "digits" in a base-α number system.

The result is unique identifier numbers, but they are so large they will quickly exceed the number of slots in our hash table (denoted by m). We must reduce this number to an integer between 0 and $m-1$, by taking the remainder of $H(S)$ mod m. This works on the same principle as a roulette wheel. The ball travels a long distance around and around the circumference-m wheel $\lfloor H(S)/m \rfloor$ times before settling down to a random bin. If the table size is selected with enough finesse (ideally m is a large prime not too close to $2^i - 1$), the resulting hash values should be fairly uniformly distributed.

3.7.1 Collision Resolution

No matter how good our hash function is, we had better be prepared for collisions, because two distinct keys will occasionally hash to the same value. *Chaining* is the easiest approach to collision resolution. Represent the hash table as an array of m linked lists, as shown in Figure 3.9. The ith list will contain all the items that hash to the value of i. Thus search, insertion, and deletion reduce to the corresponding problem in linked lists. If the n keys are distributed uniformly in a table, each list will contain roughly n/m elements, making them a constant size when $m \approx n$.

Chaining is very natural, but devotes a considerable amount of memory to pointers. This is space that could be used to make the table larger, and hence the "lists" smaller.

The alternative is something called *open addressing*. The hash table is maintained as an array of elements (not buckets), each initialized to null, as shown in Figure 3.10. On an insertion, we check to see if the desired position is empty. If so,

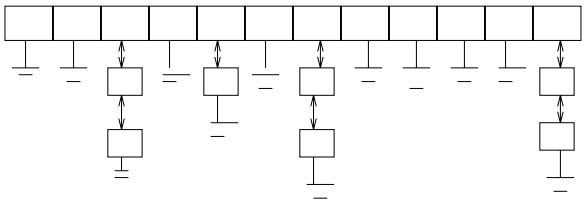

Figure 3.9: Collision resolution by chaining

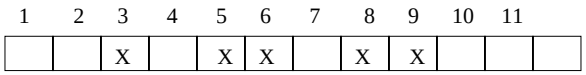

Figure 3.10: Collision resolution by open addressing

we insert it. If not, we must find some other place to insert it instead. The simplest possibility (called *sequential probing*) inserts the item in the next open spot in the table. If the table is not too full, the contiguous runs of items should be fairly small, hence this location *should* be only a few slots from its intended position.

Searching for a given key now involves going to the appropriate hash value and checking to see if the item there is the one we want. If so, return it. Otherwise we must keep checking through the length of the run.

Deletion in an open addressing scheme can get ugly, since removing one element might break a chain of insertions, making some elements inaccessible. We have no alternative but to reinsert all the items in the run following the new hole.

Chaining and open addressing both require $O(m)$ to initialize an m-element hash table to null elements prior to the first insertion. Traversing all the elements in the table takes $O(n+m)$ time for chaining, because we have to scan all m buckets looking for elements, even if the actual number of inserted items is small. This reduces to $O(m)$ time for open addressing, since n must be at most m.

When using chaining with doubly-linked lists to resolve collisions in an m-element hash table, the dictionary operations for n items can be implemented in the following expected and worst case times:

	Hash table (expected)	Hash table (worst case)
Search(L, k)	$O(n/m)$	$O(n)$
Insert(L, x)	$O(1)$	$O(1)$
Delete(L, x)	$O(1)$	$O(1)$
Successor(L, x)	$O(n+m)$	$O(n+m)$
Predecessor(L, x)	$O(n+m)$	$O(n+m)$
Minimum(L)	$O(n+m)$	$O(n+m)$
Maximum(L)	$O(n+m)$	$O(n+m)$

Pragmatically, a hash table is often the best data structure to maintain a dictionary. The applications of hashing go far beyond dictionaries, however, as we will see below.

3.7.2 Efficient String Matching via Hashing

Strings are sequences of characters where the order of the characters matters, since *ALGORITHM* is different than *LOGARITHM*. Text strings are fundamental to a host of computing applications, from programming language parsing/compilation, to web search engines, to biological sequence analysis.

The primary data structure for representing strings is an array of characters. This allows us constant-time access to the ith character of the string. Some auxiliary information must be maintained to mark the end of the string—either a special end-of-string character or (perhaps more usefully) a count of the n characters in the string.

The most fundamental operation on text strings is substring search, namely:

Problem: Substring Pattern Matching
Input: A text string t and a pattern string p.
Output: Does t contain the pattern p as a substring, and if so where?

The simplest algorithm to search for the presence of pattern string p in text t overlays the pattern string at every position in the text, and checks whether every pattern character matches the corresponding text character. As demonstrated in Section 2.5.3 (page 43), this runs in $O(nm)$ time, where $n = |t|$ and $m = |p|$.

This quadratic bound is worst-case. More complicated, worst-case linear-time search algorithms do exist: see Section 18.3 (page 628) for a complete discussion. But here we give a linear *expected-time* algorithm for string matching, called the Rabin-Karp algorithm. It is based on hashing. Suppose we compute a given hash function on both the pattern string p and the m-character substring starting from the ith position of t. If these two strings are identical, clearly the resulting hash values must be the same. If the two strings are different, the hash values will *almost certainly* be different. These false positives should be so rare that we can easily spend the $O(m)$ time it takes to explicitly check the identity of two strings whenever the hash values agree.

This reduces string matching to $n-m+2$ hash value computations (the $n-m+1$ windows of t, plus one hash of p), plus what *should be* a very small number of $O(m)$ time verification steps. The catch is that it takes $O(m)$ time to compute a hash function on an m-character string, and $O(n)$ such computations seems to leave us with an $O(mn)$ algorithm again.

But let's look more closely at our previously defined hash function, applied to the m characters starting from the jth position of string S:

$$H(S, j) = \sum_{i=0}^{m-1} \alpha^{m-(i+1)} \times char(s_{i+j})$$

What changes if we now try to compute $H(S, j+1)$—the hash of the next window of m characters? Note that $m-1$ characters are the same in both windows, although this differs by one in the number of times they are multiplied by α. A little algebra reveals that

$$H(S, j+1) = \alpha(H(S, j) - \alpha^{m-1} char(s_j)) + char(s_{j+m})$$

This means that once we know the hash value from the j position, we can find the hash value from the $(j+1)$st position for the cost of two multiplications, one addition, and one subtraction. This can be done in constant time (the value of α^{m-1} can be computed once and used for all hash value computations). This math works even if we compute $H(S, j)$ mod M, where M is a reasonably large prime number, thus keeping the size of our hash values small (at most M) even when the pattern string is long.

Rabin-Karp is a good example of a randomized algorithm (if we pick M in some random way). We get no guarantee the algorithm runs in $O(n+m)$ time, because we may get unlucky and have the hash values regularly collide with spurious matches. Still, the odds are heavily in our favor—if the hash function returns values uniformly from 0 to $M-1$, the probability of a false collision should be $1/M$. This is quite reasonable: if $M \approx n$, there should only be one false collision per string, and if $M \approx n^k$ for $k \geq 2$, the odds are great we will never see any false collisions.

3.7.3 Duplicate Detection Via Hashing

The key idea of hashing is to represent a large object (be it a key, a string, or a substring) using a single number. The goal is a representation of the large object by an entity that can be manipulated in constant time, such that it is relatively unlikely that two different large objects map to the same value.

Hashing has a variety of clever applications beyond just speeding up search. I once heard Udi Manber—then Chief Scientist at Yahoo—talk about the algorithms employed at his company. The three most important algorithms at Yahoo, he said, were hashing, hashing, and hashing.

Consider the following problems with nice hashing solutions:

- *Is a given document different from all the rest in a large corpus?* – A search engine with a huge database of n documents spiders yet another webpage. How can it tell whether this adds something new to add to the database, or is just a duplicate page that exists elsewhere on the Web?

  Explicitly comparing the new document D to all n documents is hopelessly inefficient for a large corpus. But we can hash D to an integer, and compare it to the hash codes of the rest of the corpus. Only when there is a collision is D a possible duplicate. Since we expect few spurious collisions, we can explicitly compare the few documents sharing the exact hash code with little effort.

- *Is part of this document plagiarized from a document in a large corpus?* – A lazy student copies a portion of a Web document into their term paper. "The Web is a big place," he smirks. "How will anyone ever find which one?"

  This is a more difficult problem than the previous application. Adding, deleting, or changing even one character from a document will completely change its hash code. Thus the hash codes produced in the previous application cannot help for this more general problem.

  However, we *could* build a hash table of all overlapping windows (substrings) of length w in all the documents in the corpus. Whenever there is a match of hash codes, there is likely a common substring of length w between the two documents, which can then be further investigated. We should choose w to be long enough so such a co-occurrence is very unlikely to happen by chance.

  The biggest downside of this scheme is that the size of the hash table becomes as large as the documents themselves. Retaining a small but well-chosen subset of these hash codes (say those which are exact multiples of 100) for each document leaves us likely to detect sufficiently long duplicate strings.

- *How can I convince you that a file isn't changed?* – In a closed-bid auction, each party submits their bid in secret before the announced deadline. If you knew what the other parties were bidding, you could arrange to bid \$1 more than the highest opponent and walk off with the prize as cheaply as possible. Thus the "right" auction strategy is to hack into the computer containing the bids just prior to the deadline, read the bids, and then magically emerge the winner.

  How can this be prevented? What if everyone submits a hash code of their actual bid prior to the deadline, and then submits the full bid after the deadline? The auctioneer will pick the largest full bid, but checks to make sure the hash code matches that submitted prior to the deadline. Such *cryptographic hashing* methods provide a way to ensure that the file you give me today is the same as original, because any changes to the file will result in changing the hash code.

Although the worst-case bounds on anything involving hashing are dismal, with a proper hash function we can confidently expect good behavior. Hashing is a fundamental idea in randomized algorithms, yielding linear expected-time algorithms for problems otherwise $\Theta(n \log n)$, or $\Theta(n^2)$ in the worst case.

3.8 Specialized Data Structures

The basic data structures described thus far all represent an unstructured set of items so as to facilitate retrieval operations. These data structures are well known to most programmers. Not as well known are data structures for representing more

structured or specialized kinds of objects, such as points in space, strings, and graphs.

The design principles of these data structures are the same as for basic objects. There exists a set of basic operations we need to perform repeatedly. We seek a data structure that supports these operations very efficiently. These efficient, specialized data structures are important for efficient graph and geometric algorithms so one should be aware of their existence. Details appear throughout the catalog.

- *String data structures* – Character strings are typically represented by arrays of characters, perhaps with a special character to mark the end of the string. Suffix trees/arrays are special data structures that preprocess strings to make pattern matching operations faster. See Section 12.3 (page 377) for details.

- *Geometric data structures* – Geometric data typically consists of collections of data points and regions. Regions in the plane can be described by polygons, where the boundary of the polygon is given by a chain of line segments. Polygons can be represented using an array of points $(v_1, \ldots, v_n, v_1)$, such that (v_i, v_{i+1}) is a segment of the boundary. Spatial data structures such as *kd*-trees organize points and regions by geometric location to support fast search. For more details, see Section 12.6 (page 389).

- *Graph data structures* – Graphs are typically represented using either adjacency matrices or adjacency lists. The choice of representation can have a substantial impact on the design of the resulting graph algorithms, as discussed in Chapter 6 and in the catalog in Section 12.4.

- *Set data structures* – Subsets of items are typically represented using a dictionary to support fast membership queries. Alternately, *bit vectors* are boolean arrays such that the ith bit represents true if i is in the subset. Data structures for manipulating sets is presented in the catalog in Section 12.5. The union-find data structure for maintaining set partitions will be covered in Section 6.1.3 (page 198).

3.9 War Story: String 'em Up

The human genome encodes all the information necessary to build a person. This project has already had an enormous impact on medicine and molecular biology. Algorists have become interested in the human genome project as well, for several reasons:

- DNA sequences can be accurately represented as strings of characters on the four-letter alphabet (A,C,T,G). Biologist's needs have sparked new interest in old algorithmic problems such as string matching (see Section 18.3 (page 628)) as well as creating new problems such as shortest common superstring (see Section 18.9 (page 654)).

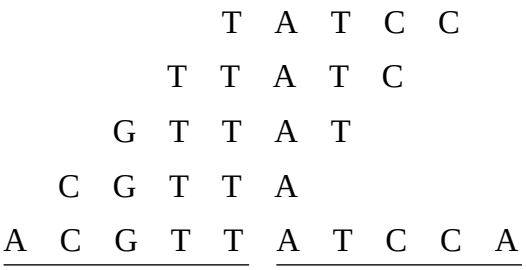

Figure 3.11: The concatenation of two fragments can be in S only if all sub-fragments are

- DNA sequences are very *long* strings. The human genome is approximately three billion base pairs (or characters) long. Such large problem size means that asymptotic (Big-Oh) complexity analysis is usually fully justified on biological problems.

- Enough money is being invested in genomics for computer scientists to want to claim their piece of the action.

One of my interests in computational biology revolved around a proposed technique for DNA sequencing called sequencing by hybridization (SBH). This procedure attaches a set of probes to an array, forming a *sequencing chip*. Each of these probes determines whether or not the probe string occurs as a substring of the DNA target. The target DNA can now be sequenced based on the constraints of which strings are (and are not) substrings of the target.

We sought to identify all the strings of length $2k$ that are possible substrings of an unknown string S, given the set of all length k substrings of S. For example, suppose we know that AC, CA, and CC are the only length-2 substrings of S. It is possible that $ACCA$ is a substring of S, since the center substring is one of our possibilities. However, $CAAC$ *cannot* be a substring of S, since AA is not a substring of S. We needed to find a fast algorithm to construct all the consistent length-$2k$ strings, since S could be very long.

The simplest algorithm to build the $2k$ strings would be to concatenate all $O(n^2)$ pairs of k-strings together, and then test to make sure that all $(k-1)$ length-k substrings spanning the boundary of the concatenation were in fact substrings, as shown in Figure 3.11. For example, the nine possible concatenations of AC, CA, and CC are $ACAC$, $ACCA$, $ACCC$, $CAAC$, $CACA$, $CACC$, $CCAC$, $CCCA$, and $CCCC$. Only $CAAC$ can be eliminated because of the absence of AA.

We needed a fast way of testing whether the $k-1$ substrings straddling the concatenation were members of our dictionary of permissible k-strings. The time it takes to do this depends upon which dictionary data structure we use. A binary search tree could find the correct string within $O(\log n)$ comparisons, where each

comparison involved testing which of two length-k strings appeared first in alphabetical order. The total time using such a binary search tree would be $O(k \log n)$.

That seemed pretty good. So my graduate student, Dimitris Margaritis, used a binary search tree data structure for our implementation. It worked great up until the moment we ran it.

"I've tried the fastest computer in our department, but our program is too slow," Dimitris complained. "It takes forever on string lengths of only 2,000 characters. We will never get up to 50,000."

We profiled our program and discovered that almost all the time was spent searching in this data structure. This was no surprise since we did this $k-1$ times for each of the $O(n^2)$ possible concatenations. We needed a faster dictionary data structure, since search was the innermost operation in such a deep loop.

"How about using a hash table?" I suggested. "It should take $O(k)$ time to hash a k-character string and look it up in our table. That should knock off a factor of $O(\log n)$, which will mean something when $n \approx 2{,}000$."

Dimitris went back and implemented a hash table implementation for our dictionary. Again, it worked great up until the moment we ran it.

"Our program is still too slow," Dimitris complained. "Sure, it is now about ten times faster on strings of length 2,000. So now we can get up to about 4,000 characters. Big deal. We will never get up to 50,000."

"We should have expected this," I mused. "After all, $\lg_2(2,000) \approx 11$. We need a faster data structure to search in our dictionary of strings."

"But what can be faster than a hash table?" Dimitris countered. "To look up a k-character string, you must read all k characters. Our hash table already does $O(k)$ searching."

"Sure, it takes k comparisons to test the first substring. But maybe we can do better on the second test. Remember where our dictionary queries are coming from. When we concatenate $ABCD$ with $EFGH$, we are first testing whether $BCDE$ is in the dictionary, then $CDEF$. These strings differ from each other by only one character. We should be able to exploit this so each subsequent test takes constant time to perform. . . ."

"We can't do that with a hash table," Dimitris observed. "The second key is not going to be anywhere near the first in the table. A binary search tree won't help, either. Since the keys $ABCD$ and $BCDE$ differ according to the first character, the two strings will be in different parts of the tree."

"But we can use a suffix tree to do this," I countered. "A suffix tree is a trie containing all the suffixes of a given set of strings. For example, the suffixes of $ACAC$ are $\{ACAC, CAC, AC, C\}$. Coupled with suffixes of string $CACT$, we get the suffix tree of Figure 3.12. By following a pointer from $ACAC$ to its longest proper suffix CAC, we get to the right place to test whether $CACT$ is in our set of strings. One character comparison is all we need to do from there."

Suffix trees are amazing data structures, discussed in considerably more detail in Section 12.3 (page 377). Dimitris did some reading about them, then built a nice

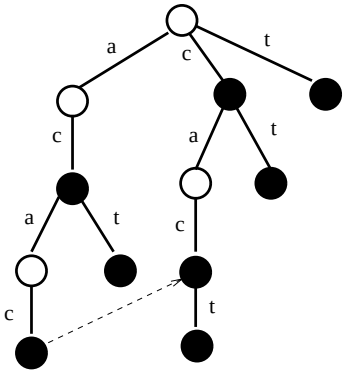

Figure 3.12: Suffix tree on $ACAC$ and $CACT$, with the pointer to the suffix of $ACAC$

suffix tree implementation for our dictionary. Once again, it worked great up until the moment we ran it.

"Now our program is faster, but it runs out of memory," Dimitris complained. "The suffix tree builds a path of length k for each suffix of length k, so all told there can be $\Theta(n^2)$ nodes in the tree. It crashes when we go beyond 2,000 characters. We will never get up to strings with 50,000 characters."

I wasn't ready to give up yet. "There is a way around the space problem, by using compressed suffix trees," I recalled. "Instead of explicitly representing long paths of character nodes, we can refer back to the original string." Compressed suffix trees always take linear space, as described in Section 12.3 (page 377).

Dimitris went back one last time and implemented the compressed suffix tree data structure. *Now* it worked great! As shown in Figure 3.13, we ran our simulation for strings of length $n = 65{,}536$ without incident. Our results showed that interactive SBH could be a very efficient sequencing technique. Based on these simulations, we were able to arouse interest in our technique from biologists. Making the actual wet laboratory experiments feasible provided another computational challenge, which is reported in Section 7.7 (page 263).

The take-home lessons for programmers from Figure 3.13 should be apparent. We isolated a single operation (dictionary string search) that was being performed repeatedly and optimized the data structure we used to support it. We started with a simple implementation (binary search trees) in the hopes that it would suffice, and then used profiling to reveal the trouble when it didn't. When an improved dictionary structure still did not suffice, we looked deeper into the kind of queries we were performing, so that we could identify an even better data structure. Finally, we didn't give up until we had achieved the level of performance we needed. In algorithms, as in life, persistence usually pays off.

String length	Binary tree	Hash table	Suffix tree	Compressed tree
8	0.0	0.0	0.0	0.0
16	0.0	0.0	0.0	0.0
32	0.1	0.0	0.0	0.0
64	0.3	0.4	0.3	0.0
128	2.4	1.1	0.5	0.0
256	17.1	9.4	3.8	0.2
512	31.6	67.0	6.9	1.3
1,024	1,828.9	96.6	31.5	2.7
2,048	11,441.7	941.7	553.6	39.0
4,096	$>$ 2 days	5,246.7	out of	45.4
8,192		$>$ 2 days	memory	642.0
16,384				1,614.0
32,768				13,657.8
65,536				39,776.9

Figure 3.13: Run times (in seconds) for the SBH simulation using various data structures

Chapter Notes

Optimizing hash table performance is surprisingly complicated for such a conceptually simple data structure. The importance of short runs in open addressing has to more sophisticated schemes than sequential probing for optimal hash table performance. For more details, see Knuth [Knu98].

Our triangle strip optimizing program, *stripe*, is described in [ESV96]. Hashing techniques for plagiarism detection are discussed in [SWA03].

Surveys of algorithmic issues in DNA sequencing by hybridization include [CK94, PL94]. Our work on interactive SBH reported in the war story is reported in [MS95a].

3.10 Exercises

Stacks, Queues, and Lists

3-1. *[3]* A common problem for compilers and text editors is determining whether the parentheses in a string are balanced and properly nested. For example, the string (((())())() contains properly nested pairs of parentheses, which the strings)()(and ()) do not. Give an algorithm that returns true if a string contains properly nested and balanced parentheses, and false if otherwise. For full credit, identify the position of the first offending parenthesis if the string is not properly nested and balanced.

3-2. *[3]* Write a program to reverse the direction of a given singly-linked list. In other words, after the reversal all pointers should now point backwards. Your algorithm should take linear time.

3-3. *[5]* We have seen how dynamic arrays enable arrays to grow while still achieving constant-time amortized performance. This problem concerns extending dynamic arrays to let them both grow and shrink on demand.

(a) Consider an underflow strategy that cuts the array size in half whenever the array falls below half full. Give an example sequence of insertions and deletions where this strategy gives a bad amortized cost.

(b) Then, give a better underflow strategy than that suggested above, one that achieves constant amortized cost per deletion.

Trees and Other Dictionary Structures

3-4. *[3]* Design a dictionary data structure in which search, insertion, and deletion can all be processed in $O(1)$ time in the worst case. You may assume the set elements are integers drawn from a finite set $1, 2, .., n$, and initialization can take $O(n)$ time.

3-5. *[3]* Find the overhead fraction (the ratio of data space over total space) for each of the following binary tree implementations on n nodes:

(a) All nodes store data, two child pointers, and a parent pointer. The data field requires four bytes and each pointer requires four bytes.

(b) Only leaf nodes store data; internal nodes store two child pointers. The data field requires four bytes and each pointer requires two bytes.

3-6. *[5]* Describe how to modify any balanced tree data structure such that search, insert, delete, minimum, and maximum still take $O(\log n)$ time each, but successor and predecessor now take $O(1)$ time each. Which operations have to be modified to support this?

3-7. *[5]* Suppose you have access to a balanced dictionary data structure, which supports each of the operations search, insert, delete, minimum, maximum, successor, and predecessor in $O(\log n)$ time. Explain how to modify the insert and delete operations so they still take $O(\log n)$ but now minimum and maximum take $O(1)$ time. (Hint: think in terms of using the abstract dictionary operations, instead of mucking about with pointers and the like.)

3-8. *[6]* Design a data structure to support the following operations:

- *insert(x,T)* – Insert item x into the set T.
- *delete(k,T)* – Delete the kth smallest element from T.
- *member(x,T)* – Return true iff $x \in T$.

All operations must take $O(\log n)$ time on an n-element set.

3-9. *[8]* A *concatenate* operation takes two sets S_1 and S_2, where every key in S_1 is smaller than any key in S_2, and merges them together. Give an algorithm to concatenate two binary search trees into one binary search tree. The worst-case running time should be $O(h)$, where h is the maximal height of the two trees.

Applications of Tree Structures

3-10. *[5]* In the *bin-packing problem*, we are given n metal objects, each weighing between zero and one kilogram. Our goal is to find the smallest number of bins that will hold the n objects, with each bin holding one kilogram at most.

- The *best-fit heuristic* for bin packing is as follows. Consider the objects in the order in which they are given. For each object, place it into the partially filled bin with the smallest amount of extra room *after* the object is inserted.. If no such bin exists, start a new bin. Design an algorithm that implements the best-fit heuristic (taking as input the n weights $w_1, w_2, ..., w_n$ and outputting the number of bins used) in $O(n \log n)$ time.
- Repeat the above using the *worst-fit heuristic*, where we put the next object in the partially filled bin with the largest amount of extra room *after* the object is inserted.

3-11. *[5]* Suppose that we are given a sequence of n values $x_1, x_2, ..., x_n$ and seek to quickly answer repeated queries of the form: given i and j, find the smallest value in $x_i, \ldots, x_j$.

(a) Design a data structure that uses $O(n^2)$ space and answers queries in $O(1)$ time.

(b) Design a data structure that uses $O(n)$ space and answers queries in $O(\log n)$ time. For partial credit, your data structure can use $O(n \log n)$ space and have $O(\log n)$ query time.

3-12. *[5]* Suppose you are given an input set S of n numbers, and a black box that if given any sequence of real numbers and an integer k instantly and correctly answers whether there is a subset of input sequence whose sum is exactly k. Show how to use the black box $O(n)$ times to find a subset of S that adds up to k.

3-13. *[5]* Let $A[1..n]$ be an array of real numbers. Design an algorithm to perform any sequence of the following operations:

- *Add(i,y)* – Add the value y to the ith number.
- *Partial-sum(i)* – Return the sum of the first i numbers, i.e. $\sum_{j=1}^{i} A[j]$.

There are no insertions or deletions; the only change is to the values of the numbers. Each operation should take $O(\log n)$ steps. You may use one additional array of size n as a work space.

3-14. *[8]* Extend the data structure of the previous problem to support insertions and deletions. Each element now has both a *key* and a *value*. An element is accessed by its key. The addition operation is applied to the values, but the elements are accessed by its key. The *Partial_sum* operation is different.

- *Add(k,y)* – Add the value y to the item with key k.
- *Insert(k,y)* – Insert a new item with key k and value y.
- *Delete(k)* – Delete the item with key k.

- *Partial-sum(k)* – Return the sum of all the elements currently in the set whose key is less than y, i.e. $\sum_{x_j < y} x_i$.

The worst case running time should still be $O(n \log n)$ for any sequence of $O(n)$ operations.

3-15. *[8]* Design a data structure that allows one to search, insert, and delete an integer X in $O(1)$ time (i.e. , constant time, independent of the total number of integers stored). Assume that $1 \leq X \leq n$ and that there are $m + n$ units of space available, where m is the maximum number of integers that can be in the table at any one time. (Hint: use two arrays $A[1..n]$ and $B[1..m]$.) You are not allowed to initialize either A or B, as that would take $O(m)$ or $O(n)$ operations. This means the arrays are full of random garbage to begin with, so you must be very careful.

Implementation Projects

3-16. *[5]* Implement versions of several different dictionary data structures, such as linked lists, binary trees, balanced binary search trees, and hash tables. Conduct experiments to assess the relative performance of these data structures in a simple application that reads a large text file and reports exactly one instance of each word that appears within it. This application can be efficiently implemented by maintaining a dictionary of all distinct words that have appeared thus far in the text and inserting/reporting each word that is not found. Write a brief report with your conclusions.

3-17. *[5]* A Caesar shift (see Section 18.6 (page 641)) is a very simple class of ciphers for secret messages. Unfortunately, they can be broken using statistical properties of English. Develop a program capable of decrypting Caesar shifts of sufficiently long texts.

Interview Problems

3-18. *[3]* What method would you use to look up a word in a dictionary?

3-19. *[3]* Imagine you have a closet full of shirts. What can you do to organize your shirts for easy retrieval?

3-20. *[4]* Write a function to find the middle node of a singly-linked list.

3-21. *[4]* Write a function to compare whether two binary trees are identical. Identical trees have the same key value at each position and the same structure.

3-22. *[4]* Write a program to convert a binary search tree into a linked list.

3-23. *[4]* Implement an algorithm to reverse a linked list. Now do it without recursion.

3-24. *[5]* What is the best data structure for maintaining URLs that have been visited by a Web crawler? Give an algorithm to test whether a given URL has already been visited, optimizing both space and time.

3-25. *[4]* You are given a search string and a magazine. You seek to generate all the characters in search string by cutting them out from the magazine. Give an algorithm to efficiently determine whether the magazine contains all the letters in the search string.

3-26. *[4]* Reverse the words in a sentence—i.e., "My name is Chris" becomes "Chris is name My." Optimize for time and space.

3-27. *[5]* Determine whether a linked list contains a loop as quickly as possible without using any extra storage. Also, identify the location of the loop.

3-28. *[5]* You have an unordered array X of n integers. Find the array M containing n elements where M_i is the product of all integers in X except for X_i. You may not use division. You can use extra memory. (Hint: There are solutions faster than $O(n^2)$.)

3-29. *[6]* Give an algorithm for finding an ordered word pair (e.g., "New York") occurring with the greatest frequency in a given webpage. Which data structures would you use? Optimize both time and space.

Programming Challenges

These programming challenge problems with robot judging are available at *http://www.programming-challenges.com* or *http://online-judge.uva.es*.

3-1. "Jolly Jumpers" – Programming Challenges 110201, UVA Judge 10038.

3-2. "Crypt Kicker" – Programming Challenges 110204, UVA Judge 843.

3-3. "Where's Waldorf?" – Programming Challenges 110302, UVA Judge 10010.

3-4. "Crypt Kicker II" – Programming Challenges 110304, UVA Judge 850.

4

Sorting and Searching

Typical computer science students study the basic sorting algorithms at least three times before they graduate: first in introductory programming, then in data structures, and finally in their algorithms course. Why is sorting worth so much attention? There are several reasons:

- Sorting is the basic building block that many other algorithms are built around. By understanding sorting, we obtain an amazing amount of power to solve other problems.
- Most of the interesting ideas used in the design of algorithms appear in the context of sorting, such as divide-and-conquer, data structures, and randomized algorithms.
- Computers have historically spent more time sorting than doing anything else. A quarter of all mainframe cycles were spent sorting data [Knu98]. Sorting remains the most ubiquitous combinatorial algorithm problem in practice.
- Sorting is the most thoroughly studied problem in computer science. Literally dozens of different algorithms are known, most of which possess some particular advantage over all other algorithms in certain situations.

In this chapter, we will discuss sorting, stressing how sorting can be applied to solving other problems. In this sense, sorting behaves more like a data structure than a problem in its own right. We then give detailed presentations of several fundamental algorithms: heapsort, mergesort, quicksort, and distribution sort as examples of important algorithm design paradigms. Sorting is also represented by Section 14.1 (page 436) in the problem catalog.

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4.1 Applications of Sorting

We will review several sorting algorithms and their complexities over the course of this chapter. But the punch-line is this: clever sorting algorithms exist that run in $O(n \log n)$. This is a *big* improvement over naive $O(n^2)$ sorting algorithms for large values of n. Consider the following table:

n	$n^2/4$	$n \lg n$
10	*25*	33
100	2,500	*664*
1,000	250,000	*9,965*
10,000	25,000,000	*132,877*
100,000	2,500,000,000	*1,660,960*

You might still get away with using a quadratic-time algorithm even if $n = 10,000$, but quadratic-time sorting is clearly ridiculous once $n \geq 100,000$.

Many important problems can be reduced to sorting, so we can use our clever $O(n \log n)$ algorithms to do work that might otherwise seem to require a quadratic algorithm. An important algorithm design technique is to use sorting as a basic building block, because many other problems become easy once a set of items is sorted.

Consider the following applications:

- *Searching* – Binary search tests whether an item is in a dictionary in $O(\log n)$ time, provided the keys are all sorted. Search preprocessing is perhaps the single most important application of sorting.

- *Closest pair* – Given a set of n numbers, how do you find the pair of numbers that have the smallest difference between them? Once the numbers are sorted, the closest pair of numbers must lie next to each other somewhere in sorted order. Thus, a linear-time scan through them completes the job, for a total of $O(n \log n)$ time including the sorting.

- *Element uniqueness* – Are there any duplicates in a given set of n items? This is a special case of the closest-pair problem above, where we ask if there is a pair separated by a gap of zero. The most efficient algorithm sorts the numbers and then does a linear scan though checking all adjacent pairs.

- *Frequency distribution* – Given a set of n items, which element occurs the largest number of times in the set? If the items are sorted, we can sweep from left to right and count them, since all identical items will be lumped together during sorting.

  To find out how often an arbitrary element k occurs, look up k using binary search in a sorted array of keys. By walking to the left of this point until the first the element is not k and then doing the same to the right, we can find

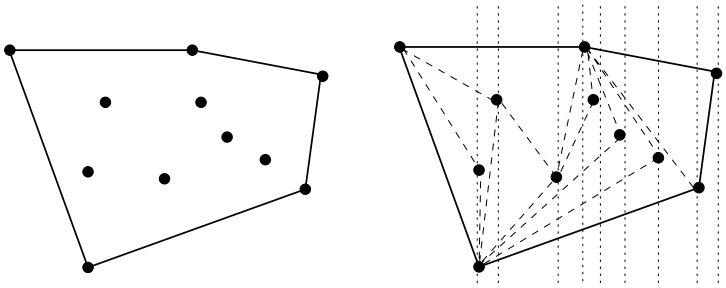

Figure 4.1: The convex hull of a set of points (l), constructed by left-to-right insertion.

this count in $O(\log n + c)$ time, where c is the number of occurrences of k. Even better, the number of instances of k can be found in $O(\log n)$ time by using binary search to look for the positions of both $k - \epsilon$ and $k + \epsilon$ (where ϵ is arbitrarily small) and then taking the difference of these positions.

- *Selection* – What is the kth largest item in an array? If the keys are placed in sorted order, the kth largest can be found in constant time by simply looking at the kth position of the array. In particular, the median element (see Section 14.3 (page 445)) appears in the $(n/2)$nd position in sorted order.

- *Convex hulls* – What is the polygon of smallest area that contains a given set of n points in two dimensions? The convex hull is like a rubber band stretched over the points in the plane and then released. It compresses to just cover the points, as shown in Figure 4.1(l). The convex hull gives a nice representation of the shape of the points and is an important building block for more sophisticated geometric algorithms, as discussed in the catalog in Section 17.2 (page 568).

  But how can we use sorting to construct the convex hull? Once you have the points sorted by x-coordinate, the points can be inserted from left to right into the hull. Since the right-most point is always on the boundary, we know that it will appear in the hull. Adding this new right-most point may cause others to be deleted, but we can quickly identify these points because they lie inside the polygon formed by adding the new point. See the example in Figure 4.1(r). These points will be neighbors of the previous point we inserted, so they will be easy to find and delete. The total time is linear after the sorting has been done.

While a few of these problems (namely median and selection) can be solved in linear time using more sophisticated algorithms, sorting provides quick and easy solutions to all of these problems. It is a rare application where the running time

of sorting proves to be the bottleneck, especially a bottleneck that could have otherwise been removed using more clever algorithmics. Never be afraid to spend time sorting, provided you use an efficient sorting routine.

Take-Home Lesson: Sorting lies at the heart of many algorithms. Sorting the data is one of the first things any algorithm designer should try in the quest for efficiency.

Stop and Think: Finding the Intersection

Problem: Give an efficient algorithm to determine whether two sets (of size m and n, respectively) are disjoint. Analyze the worst-case complexity in terms of m and n, considering the case where m is substantially smaller than n.

Solution: At least three algorithms come to mind, all of which are variants of sorting and searching:

- *First sort the big set* – The big set can be sorted in $O(n \log n)$ time. We can now do a binary search with each of the m elements in the second, looking to see if it exists in the big set. The total time will be $O((n+m)\log n)$.

- *First sort the small set* – The small set can be sorted in $O(m \log m)$ time. We can now do a binary search with each of the n elements in the big set, looking to see if it exists in the small one. The total time will be $O((n+m)\log m)$.

- *Sort both sets* – Observe that once the two sets are sorted, we no longer have to do binary search to detect a common element. We can compare the smallest elements of the two sorted sets, and discard the smaller one if they are not identical. By repeating this idea recursively on the now smaller sets, we can test for duplication in linear time after sorting. The total cost is $O(n \log n + m \log m + n + m)$.

So, which of these is the fastest method? Clearly small-set sorting trumps big-set sorting, since $\log m < \log n$ when $m < n$. Similarly, $(n+m)\log m$ must be asymptotically less than $n \log n$, since $n + m < 2n$ when $m < n$. Thus, sorting the small set is the best of these options. Note that this is linear when m is constant in size.

Note that *expected* linear time can be achieved by hashing. Build a hash table containing the elements of both sets, and verify that collisions in the same bucket are in fact identical elements. In practice, this may be the best solution. ∎

4.2 Pragmatics of Sorting

We have seen many algorithmic applications of sorting, and we will see several efficient sorting algorithms. One issue stands between them: in what order do we want our items sorted?

The answers to this basic question are application-specific. Consider the following considerations:

- *Increasing or decreasing order?* – A set of keys S are sorted in *ascending* order when $S_i \leq S_{i+1}$ for all $1 \leq i < n$. They are in *descending order* when $S_i \geq S_{i+1}$ for all $1 \leq i < n$. Different applications call for different orders.

- *Sorting just the key or an entire record?* – Sorting a data set involves maintaining the integrity of complex data records. A mailing list of names, addresses, and phone numbers may be sorted by names as the key field, but it had better retain the linkage between names and addresses. Thus, we need to specify which field is the key field in any complex record, and understand the full extent of each record.

- *What should we do with equal keys?* Elements with equal key values will all bunch together in any total order, but sometimes the relative order among these keys matters. Suppose an encyclopedia contains both Michael Jordan (the basketball player) and Michael Jordan (the statistician). Which entry should appear first? You may need to resort to secondary keys, such as article size, to resolve ties in a meaningful way.

  Sometimes it is required to leave the items in the same relative order as in the original permutation. Sorting algorithms that automatically enforce this requirement are called *stable*. Unfortunately few fast algorithms are stable. Stability can be achieved for any sorting algorithm by adding the initial position as a secondary key.

  Of course we could make no decision about equal key order and let the ties fall where they may. But beware, certain efficient sort algorithms (such as quicksort) can run into quadratic performance trouble unless explicitly engineered to deal with large numbers of ties.

- *What about non-numerical data?* – Alphabetizing is the sorting of text strings. Libraries have very complete and complicated rules concerning the relative *collating sequence* of characters and punctuation. Is *Skiena* the same key as *skiena*? Is *Brown-Williams* before or after *Brown America*, and before or after *Brown, John*?

The right way to specify such matters to your sorting algorithm is with an application-specific pairwise-element *comparison function*. Such a comparison function takes pointers to record items a and b and returns "$<$" if $a < b$, "$>$" if $a > b$, or "$=$" if $a = b$.

By abstracting the pairwise ordering decision to such a comparison function, we can implement sorting algorithms independently of such criteria. We simply pass the comparison function in as an argument to the sort procedure. Any reasonable programming language has a built-in sort routine as a library function. You are almost always better off using this than writing your own routine. For example, the standard library for C contains the `qsort` function for sorting:

```
#include <stdlib.h>

void qsort(void *base, size_t nel, size_t width,
          int (*compare) (const void *, const void *));
```

The key to using `qsort` is realizing what its arguments do. It sorts the first `nel` elements of an array (pointed to by `base`), where each element is `width`-bytes long. Thus we can sort arrays of 1-byte characters, 4-byte integers, or 100-byte records, all by changing the value of `width`.

The ultimate desired order is determined by the `compare` function. It takes as arguments pointers to two `width`-byte elements, and returns a negative number if the first belongs before the second in sorted order, a positive number if the second belongs before the first, or zero if they are the same. Here is a comparison function to sort integers in increasing order:

```
int intcompare(int *i, int *j)
{
    if (*i > *j) return (1);
    if (*i < *j) return (-1);
    return (0);
}
```

This comparison function can be used to sort an array `a`, of which the first `n` elements are occupied, as follows:

```
    qsort(a, n, sizeof(int), intcompare);
```

`qsort` suggests that quicksort is the algorithm implemented in this library function, although this is usually irrelevant to the user.

4.3 Heapsort: Fast Sorting via Data Structures

Sorting is a natural laboratory for studying algorithm design paradigms, since many useful techniques lead to interesting sorting algorithms. The next several sections will introduce algorithmic design techniques motivated by particular sorting algorithms.

The alert reader should ask why we review the standard sorting when you are better off *not* implementing them and using built-in library functions instead. The answer is that the design techniques are very important for other algorithmic problems you are likely to encounter.

We start with data structure design, because one of the most dramatic algorithmic improvements via appropriate data structures occurs in sorting. Selection sort is a simple-to-code algorithm that repeatedly extracts the smallest remaining element from the unsorted part of the set:

```
SelectionSort(A)
    For i = 1 to n do
        Sort[i] = Find-Minimum from A
        Delete-Minimum from A
    Return(Sort)
```

A C language implementation of selection sort appeared back in Section 2.5.1 (page 41). There we partitioned the input array into sorted and unsorted regions. To find the smallest item, we performed a linear sweep through the unsorted portion of the array. The smallest item is then swapped with the ith item in the array before moving on to the next iteration. Selection sort performs n iterations, where the average iteration takes $n/2$ steps, for a total of $O(n^2)$ time.

But what if we improve the data structure? It takes $O(1)$ time to remove a particular item from an unsorted array once it has been located, but $O(n)$ time to find the smallest item. These are exactly the operations supported by priority queues. So what happens if we replace the data structure with a better priority queue implementation, either a heap or a balanced binary tree? Operations within the loop now take $O(\log n)$ time each, instead of $O(n)$. Using such a priority queue implementation speeds up selection sort from $O(n^2)$ to $O(n \log n)$.

The name typically given to this algorithm, *heapsort*, obscures the relationship between them, but heapsort is nothing but an implementation of selection sort using the right data structure.

4.3.1 Heaps

Heaps are a simple and elegant data structure for efficiently supporting the priority queue operations insert and extract-min. They work by maintaining a partial order on the set of elements which is weaker than the sorted order (so it can be efficient to maintain) yet stronger than random order (so the minimum element can be quickly identified).

Power in any hierarchically-structured organization is reflected by a tree, where each node in the tree represents a person, and edge (x, y) implies that x directly supervises (or dominates) y. The fellow at the root sits at the "top of the heap."

In this spirit, a *heap-labeled tree* is defined to be a binary tree such that the key labeling of each node *dominates* the key labeling of each of its children. In a

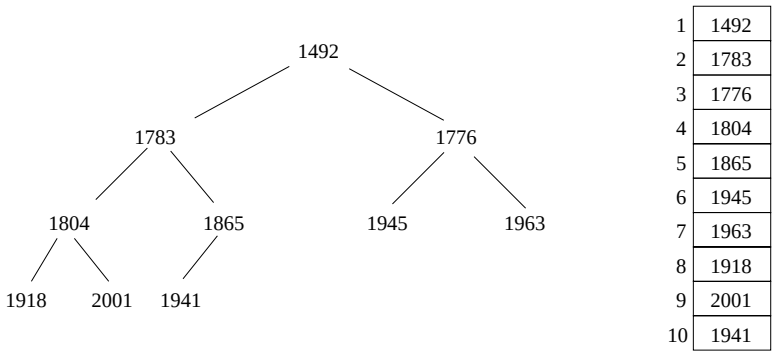

Figure 4.2: A heap-labeled tree of important years from American history (l), with the corresponding implicit heap representation (r)

min-heap, a node dominates its children by containing a smaller key than they do, while in a *max-heap* parent nodes dominate by being bigger. Figure 4.2(l) presents a min-heap ordered tree of red-letter years in American history (kudos to you if you can recall what happened each year).

The most natural implementation of this binary tree would store each key in a node with pointers to its two children. As with binary search trees, the memory used by the pointers can easily outweigh the size of keys, which is the data we are really interested in.

The heap is a slick data structure that enables us to represent binary trees without using any pointers. We will store data as an array of keys, and use the position of the keys to *implicitly* satisfy the role of the pointers.

We will store the root of the tree in the first position of the array, and its left and right children in the second and third positions, respectively. In general, we will store the 2^l keys of the lth level of a complete binary tree from left-to-right in positions 2^{l-1} to $2^l - 1$, as shown in Figure 4.2(r). We assume that the array starts with index 1 to simplify matters.

```
typedef struct {
        item_type q[PQ_SIZE+1];        /* body of queue */
        int n;                         /* number of queue elements */
} priority_queue;
```

What is especially nice about this representation is that the positions of the parent and children of the key at position k are readily determined. The *left* child of k sits in position $2k$ and the right child in $2k + 1$, while the parent of k holds court in position $\lfloor n/2 \rfloor$. Thus we can move around the tree without any pointers.

```
pq_parent(int n)
{
        if (n == 1) return(-1);
        else return((int) n/2);     /* implicitly take floor(n/2) */
}

pq_young_child(int n)
{
        return(2 * n);
}
```

So, we can store any binary tree in an array without pointers. What is the catch? Suppose our height h tree was sparse, meaning that the number of nodes $n < 2^h$. All missing internal nodes still take up space in our structure, since we must represent a full binary tree to maintain the positional mapping between parents and children.

Space efficiency thus demands that we not allow holes in our tree—i.e., that each level be packed as much as it can be. If so, only the last level may be incomplete. By packing the elements of the last level as far to the left as possible, we can represent an n-key tree using exactly n elements of the array. If we did not enforce these structural constraints, we might need an array of size 2^n to store the same elements. Since all but the last level is always filled, the height h of an n element heap is logarithmic because:

$$\sum_{i=0}^{h} 2^i = 2^{h+1} - 1 \geq n$$

so $h = \lfloor \lg n \rfloor$.

This implicit representation of binary trees saves memory, but is less flexible than using pointers. We cannot store arbitrary tree topologies without wasting large amounts of space. We cannot move subtrees around by just changing a single pointer, only by explicitly moving each of the elements in the subtree. This loss of flexibility explains why we cannot use this idea to represent binary search trees, but it works just fine for heaps.

Stop and Think: Who's where in the heap?

Problem: How can we efficiently search for a particular key in a heap?

Solution: We can't. Binary search does not work because a heap is not a binary search tree. We know almost nothing about the relative order of the $n/2$ leaf elements in a heap—certainly nothing that lets us avoid doing linear search through them. ∎

4.3.2 Constructing Heaps

Heaps can be constructed incrementally, by inserting each new element into the left-most open spot in the array, namely the $(n+1)$st position of a previously n-element heap. This ensures the desired balanced shape of the heap-labeled tree, but does not necessarily maintain the dominance ordering of the keys. The new key might be less than its parent in a min-heap, or greater than its parent in a max-heap.

The solution is to swap any such dissatisfied element with its parent. The old parent is now happy, because it is properly dominated. The other child of the old parent is still happy, because it is now dominated by an element even more extreme than its previous parent. The new element is now happier, but may still dominate its new parent. We now recur at a higher level, *bubbling up* the new key to its proper position in the hierarchy. Since we replace the root of a subtree by a larger one at each step, we preserve the heap order elsewhere.

```
pq_insert(priority_queue *q, item_type x)
{
  if (q->n >= PQ_SIZE)
         printf("Warning: priority queue overflow insert x=%d\n",x);
  else {
         q->n = (q->n) + 1;
         q->q[ q->n ] = x;
         bubble_up(q, q->n);
  }
}

bubble_up(priority_queue *q, int p)
{
    if (pq_parent(p) == -1) return; /* at root of heap, no parent */

    if (q->q[pq_parent(p)] > q->q[p]) {
           pq_swap(q,p,pq_parent(p));
           bubble_up(q, pq_parent(p));
    }
}
```

This swap process takes constant time at each level. Since the height of an n-element heap is $\lfloor \lg n \rfloor$, each insertion takes at most $O(\log n)$ time. Thus an initial heap of n elements can be constructed in $O(n \log n)$ time through n such insertions:

```
pq_init(priority_queue *q)
{
        q->n = 0;
}
```

```
make_heap(priority_queue *q, item_type s[], int n)
{
        int i;                          /* counter */

        pq_init(q);
        for (i=0; i<n; i++)
                pq_insert(q, s[i]);
}
```

4.3.3 Extracting the Minimum

The remaining priority queue operations are identifying and deleting the dominant element. Identification is easy, since the top of the heap sits in the first position of the array.

Removing the top element leaves a hole in the array. This can be filled by moving the element from the *right-most* leaf (sitting in the nth position of the array) into the first position.

The shape of the tree has been restored but (as after insertion) the labeling of the root may no longer satisfy the heap property. Indeed, this new root may be dominated by both of its children. The root of this min-heap should be the smallest of three elements, namely the current root and its two children. If the current root is dominant, the heap order has been restored. If not, the dominant child should be swapped with the root and the problem pushed down to the next level.

This dissatisfied element *bubbles down* the heap until it dominates all its children, perhaps by becoming a leaf node and ceasing to have any. This percolate-down operation is also called *heapify*, because it merges two heaps (the subtrees below the original root) with a new key.

```
item_type extract_min(priority_queue *q)
{
        int min = -1;                   /* minimum value */

        if (q->n <= 0) printf("Warning: empty priority queue.\n");
        else {
                min = q->q[1];

                q->q[1] = q->q[ q->n ];
                q->n = q->n - 1;
                bubble_down(q,1);
        }

        return(min);
}
```

```
bubble_down(priority_queue *q, int p)
{
        int c;                          /* child index */
        int i;                          /* counter */
        int min_index;                  /* index of lightest child */

        c = pq_young_child(p);
        min_index = p;

        for (i=0; i<=1; i++)
                if ((c+i) <= q->n) {
                   if (q->q[min_index] > q->q[c+i]) min_index = c+i;
                }

        if (min_index != p) {
                pq_swap(q,p,min_index);
                bubble_down(q, min_index);
        }
}
```

We will reach a leaf after $\lfloor \lg n \rfloor$ `bubble_down` steps, each constant time. Thus root deletion is completed in $O(\log n)$ time.

Exchanging the maximum element with the last element and calling heapify repeatedly gives an $O(n \log n)$ sorting algorithm, named *Heapsort*.

```
heapsort(item_type s[], int n)
{
        int i;                  /* counters */
        priority_queue q;       /* heap for heapsort */

        make_heap(&q,s,n);

        for (i=0; i<n; i++)
                s[i] = extract_min(&q);
}
```

Heapsort is a great sorting algorithm. It is simple to program; indeed, the complete implementation has been presented above. It runs in worst-case $O(n \log n)$ time, which is the best that can be expected from any sorting algorithm. It is an *in-place* sort, meaning it uses no extra memory over the array containing the elements to be sorted. Although other algorithms prove slightly faster in practice, you won't go wrong using heapsort for sorting data that sits in the computer's main memory.

Priority queues are very useful data structures. Recall they were the hero of the war story described in Section 3.6 (page 85). A complete set of priority queue implementations is presented in catalog Section 12.2 (page 373).

4.3.4 Faster Heap Construction (*)

As we have seen, a heap can be constructed on n elements by incremental insertion in $O(n \log n)$ time. Surprisingly, heaps can be constructed even faster by using our `bubble_down` procedure and some clever analysis.

Suppose we pack the n keys destined for our heap into the first n elements of our priority-queue array. The shape of our heap will be right, but the dominance order will be all messed up. How can we restore it?

Consider the array in reverse order, starting from the last (nth) position. It represents a leaf of the tree and so dominates its nonexistent children. The same is the case for the last $n/2$ positions in the array, because all are leaves. If we continue to walk backwards through the array we will finally encounter an internal node with children. This element may not dominate its children, but its children represent well-formed (if small) heaps.

This is exactly the situation the `bubble_down` procedure was designed to handle, restoring the heap order of arbitrary root element sitting on top of two sub-heaps. Thus we can create a heap by performing $n/2$ non-trivial calls to the `bubble_down` procedure:

```
make_heap(priority_queue *q, item_type s[], int n)
{
        int i;                          /* counter */

        q->n = n;
        for (i=0; i<n; i++) q->q[i+1] = s[i];

        for (i=q->n; i>=1; i--) bubble_down(q,i);
}
```

Multiplying the number of calls to `bubble_down` (n) times an upper bound on the cost of each operation ($O(\log n)$) gives us a running time analysis of $O(n \log n)$. This would make it no faster than the incremental insertion algorithm described above.

But note that it is indeed an *upper bound*, because only the last insertion will actually take $\lfloor \lg n \rfloor$ steps. Recall that `bubble_down` takes time proportional to the height of the heaps it is merging. Most of these heaps are extremely small. In a full binary tree on n nodes, there are $n/2$ nodes that are leaves (i.e. , height 0), $n/4$

nodes that are height 1, $n/8$ nodes that are height 2, and so on. In general, there are at most $\lceil n/2^{h+1} \rceil$ nodes of height h, so the cost of building a heap is:

$$\sum_{h=0}^{\lfloor \lg n \rfloor} \lceil n/2^{h+1} \rceil h \leq n \sum_{h=0}^{\lfloor \lg n \rfloor} h/2^h \leq 2n$$

Since this sum is not quite a geometric series, we can't apply the usual identity to get the sum, but rest assured that the puny contribution of the numerator (h) is crushed by the denominator (2^h). The series quickly converges to linear.

Does it matter that we can construct heaps in linear time instead of $O(n \log n)$? Usually not. The construction time did not dominate the complexity of heapsort, so improving the construction time does not improve its worst-case performance. Still, it is an impressive display of the power of careful analysis, and the free lunch that geometric series convergence can sometimes provide.

Stop and Think: Where in the Heap?

Problem: Given an array-based heap on n elements and a real number x, efficiently determine whether the kth smallest element in the heap is greater than or equal to x. Your algorithm should be $O(k)$ in the worst-case, independent of the size of the heap. Hint: you do not have to find the kth smallest element; you need only determine its relationship to x.

Solution: There are at least two different ideas that lead to correct but inefficient algorithms for this problem:

1. Call extract-min k times, and test whether all of these are less than x. This explicitly sorts the first k elements and so gives us more information than the desired answer, but it takes $O(k \log n)$ time to do so.

2. The kth smallest element cannot be deeper than the kth level of the heap, since the path from it to the root must go through elements of decreasing value. Thus we can look at all the elements on the first k levels of the heap, and count how many of them are less than x, stopping when we either find k of them or run out of elements. This is correct, but takes $O(\min(n, 2^k))$ time, since the top k elements have 2^k elements.

An $O(k)$ solution can look at only k elements smaller than x, plus at most $O(k)$ elements greater than x. Consider the following recursive procedure, called at the root with $i = 1$ with $count = k$:

```
int heap_compare(priority_queue *q, int i, int count, int x)
{
        if ((count <= 0) || (i > q->n) return(count);

        if (q->q[i] < x) {
            count = heap_compare(q, pq_young_child(i), count-1, x);
            count = heap_compare(q, pq_young_child(i)+1, count, x);
        }

        return(count);
}
```

If the root of the min-heap is $\geq x$, then no elements in the heap can be less than x, as by definition the root must be the smallest element. This procedure searches the children of all nodes of weight smaller than x until either (a) we have found k of them, when it returns 0, or (b) they are exhausted, when it returns a value greater than zero. Thus it will find enough small elements if they exist.

But how long does it take? The only nodes whose children we look at are those $< x$, and at most k of these in total. Each have at most visited two children, so we visit at most $3k$ nodes, for a total time of $O(k)$. ∎

4.3.5 Sorting by Incremental Insertion

Now consider a different approach to sorting via efficient data structures. Select an arbitrary element from the unsorted set, and put it in the proper position in the sorted set.

```
InsertionSort(A)
    A[0] = -∞
    for i = 2 to n do
        j = i
        while (A[j] < A[j - 1]) do
            swap(A[j], A[j - 1])
            j = j - 1
```

A C language implementation of insertion sort appeared in Section 2.5.2 (page 43). Although insertion sort takes $O(n^2)$ in the worst case, it performs considerably better if the data is almost sorted, since few iterations of the inner loop suffice to sift it into the proper position.

Insertion sort is perhaps the simplest example of the *incremental insertion* technique, where we build up a complicated structure on n items by first building it on $n-1$ items and then making the necessary changes to add the last item. Incremental insertion proves a particularly useful technique in geometric algorithms.

Note that faster sorting algorithms based on incremental insertion follow from more efficient data structures. Insertion into a balanced search tree takes $O(\log n)$ per operation, or a total of $O(n \log n)$ to construct the tree. An in-order traversal reads through the elements in sorted order to complete the job in linear time.

4.4 War Story: Give me a Ticket on an Airplane

I came into this particular job seeking justice. I'd been retained by an air travel company to help design an algorithm to find the cheapest available airfare from city x to city y. Like most of you, I suspect, I'd been baffled at the crazy price fluctuations of ticket prices under modern "yield management." The price of flights seems to soar far more efficiently than the planes themselves. The problem, it seemed to me, was that airlines never wanted to show the true cheapest price. By doing my job right, I could make damned sure they would show it to me next time.

"Look," I said at the start of the first meeting. "This can't be so hard. Construct a graph with vertices corresponding to airports, and add an edge between each airport pair (u, v) which shows a direct flight from u to v. Set the weight of this edge equal to the cost of the cheapest available ticket from u to v. Now the cheapest fair from x to y is given by the shortest x-y path in this graph. This path/fare can be found using Dijkstra's shortest path algorithm. Problem solved!" I announced, waiving my hand with a flourish.

The assembled cast of the meeting nodded thoughtfully, then burst out laughing. It was I who needed to learn something about the overwhelming complexity of air travel pricing. There are literally millions of different fares available at any time, with prices changing several times daily. Restrictions on the availability of a particular fare in a particular context is enforced by a complicated set of pricing rules. These rules are an industry-wide kludge—a complicated structure with little in the way of consistent logical principles, which is exactly what we would need to search efficiently for the minimum fare. My favorite rule exceptions applied only to the country of Malawi. With a population of only 12 million and per-capita income of $596 (179th in the world), they prove to be an unexpected powerhouse shaping world aviation price policy. Accurately pricing any air itinerary requires at least implicit checks to ensure the trip doesn't take us through Malawi.

Part of the real problem is that there can easily be 100 different fares for the first flight leg, say from Los Angeles (LAX) to Chicago (ORD), and a similar number for each subsequent leg, say from Chicago to New York (JFK). The cheapest possible LAX-ORD fare (maybe an AARP children's price) might not be combinable with the cheapest ORD-JFK fare (perhaps a pre-Ramadan special that can only be used with subsequent connections to Mecca).

After being properly chastised for oversimplifying the problem, I got down to work. I started by reducing the problem to the simplest interesting case. "So, you

X	Y
$100	$50
$110	$75
$130	$125

X+Y	
$150	(1,1)
$160	(2,1)
$175	(1,2)
$180	(3,1)
$185	(2,2)
$205	(2,3)
$225	(1,3)
$235	(2,3)
$255	(3,3)

Figure 4.3: Sorting the pairwise sums of lists X and Y.

need to find the cheapest two-hop fare that passes your rule tests. Is there a way to decide in advance which pairs will pass without explicitly testing them?"

"No, there is no way to tell," they assured me. "We can only consult a black box routine to decide whether a particular price is available for the given itinerary/travelers."

"So our goal is to call this black box on the fewest number of combinations. This means evaluating all possible fare combinations in order from cheapest to most expensive, and stopping as soon as we encounter the first legal combination."

"Right."

"Why not construct the $m \times n$ possible price pairs, sort them in terms of cost, and evaluate them in sorted order? Clearly this can be done in $O(nm \log(nm))$ time."[1]

"That is basically what we do now, but it is quite expensive to construct the full set of $m \times n$ pairs, since the first one might be all we need."

I caught a whiff of an interesting problem. "So what you really want is an efficient data structure to repeatedly return the *next* most expensive pair without constructing all the pairs in advance."

This was indeed an interesting problem. Finding the largest element in a set under insertion and deletion is *exactly* what priority queues are good for. The catch here is that we could not seed the priority queue with all values in advance. We had to insert new pairs into the queue after each evaluation.

I constructed some examples, like the one in Figure 4.3. We could represent each fare by the list indexes of its two components. The cheapest single fare will certainly be constructed by adding up the cheapest component from both lists,

[1]The question of whether all such sums can be sorted faster than nm arbitrary integers is a notorious open problem in algorithm theory. See [Fre76, Lam92] for more on $X + Y$ sorting, as the problem is known.

described $(1,1)$. The second cheapest fare would be made from the head of one list and the second element of another, and hence would be either $(1,2)$ or $(2,1)$. Then it gets more complicated. The third cheapest could either be the unused pair above or $(1,3)$ or $(3,1)$. Indeed it would have been $(3,1)$ in the example above if the third fare of X had been \$120.

"Tell me," I asked. "Do we have time to sort the two respective lists of fares in increasing order?"

"Don't have to." the leader replied. "They come out in sorted order from the database."

Good news. That meant there was a natural order to the pair values. We never need to evaluate the pairs $(i+1,j)$ or $(i,j+1)$ before (i,j), because they clearly define more expensive fares.

"Got it!," I said. "We will keep track of index pairs in a priority queue, with the sum of the fare costs as the key for the pair. Initially we put only pair $(1,1)$ on the queue. If it proves it is not feasible, we put its two successors on—namely $(1,2)$ and $(2,1)$. In general, we enqueue pairs $(i+1,j)$ and $(i,j+1)$ after evaluating/rejecting pair (i,j). We will get through all the pairs in the right order if we do so."

The gang caught on quickly. "Sure. But what about duplicates? We will construct pair (x,y) two different ways, both when expanding $(x-1,y)$ and $(x,y-1)$."

"You are right. We need an extra data structure to guard against duplicates. The simplest might be a hash table to tell us whether a given pair exists in the priority queue before we insert a duplicate. In fact, we will never have more than n active pairs in our data structure, since there can only be one pair for each distinct value of the first coordinate."

And so it went. Our approach naturally generalizes to itineraries with more than two legs, (a complexity which grows with the number of legs). The best-first evaluation inherent in our priority queue enabled the system to stop as soon as it found the provably cheapest fare. This proved to be fast enough to provide interactive response to the user. That said, I haven't noticed my travel tickets getting any cheaper.

4.5 Mergesort: Sorting by Divide-and-Conquer

Recursive algorithms reduce large problems into smaller ones. A recursive approach to sorting involves partitioning the elements into two groups, sorting each of the smaller problems recursively, and then interleaving the two sorted lists to totally order the elements. This algorithm is called *mergesort*, recognizing the importance of the interleaving operation:

Mergesort$(A[1,n])$
    Merge(MergeSort$(A[1,\lfloor n/2 \rfloor])$, MergeSort$(A[\lfloor n/2 \rfloor + 1, n])$)

The basis case of the recursion occurs when the subarray to be sorted consists of a single element, so no rearrangement is possible. A trace of the execution of

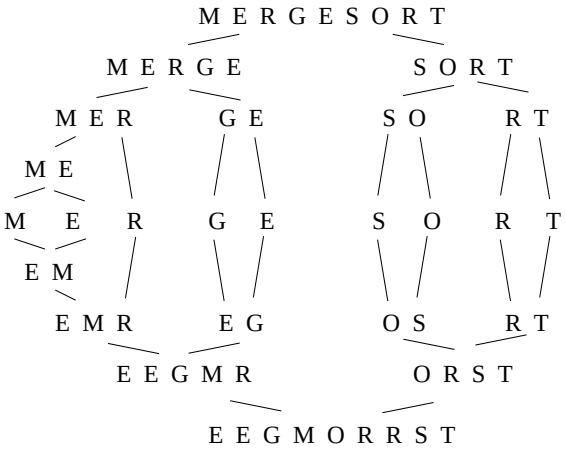

Figure 4.4: Animation of mergesort in action

mergesort is given in Figure 4.4. Picture the action as it happens during an in-order traversal of the top tree, with the array-state transformations reported in the bottom, reflected tree.

The efficiency of mergesort depends upon how efficiently we combine the two sorted halves into a single sorted list. We could concatenate them into one list and call heapsort or some other sorting algorithm to do it, but that would just destroy all the work spent sorting our component lists.

Instead we can *merge* the two lists together. Observe that the smallest overall item in two lists sorted in increasing order (as above) must sit at the top of one of the two lists. This smallest element can be removed, leaving two sorted lists behind—one slightly shorter than before. The second smallest item overall must be atop one of these lists. Repeating this operation until both lists are empty merges two sorted lists (with a total of n elements between them) into one, using at most $n-1$ comparisons or $O(n)$ total work.

What is the total running time of mergesort? It helps to think about how much work is done at each level of the execution tree. If we assume for simplicity that n is a power of two, the kth level consists of all the 2^k calls to `mergesort` processing subranges of $n/2^k$ elements.

The work done on the $(k=0)$th level involves merging two sorted lists, each of size $n/2$, for a total of at most $n-1$ comparisons. The work done on the $(k=1)$th level involves merging two pairs of sorted lists, each of size $n/4$, for a total of at most $n-2$ comparisons. In general, the work done on the kth level involves merging 2^k pairs sorted list, each of size $n/2^{k+1}$, for a total of at most $n-2^k$ comparisons. *Linear work is done merging all the elements on each level.* Each of the n elements

appears in exactly one subproblem on each level. The most expensive case (in terms of comparsions) is actually the top level.

The number of elements in a subproblem gets halved at each level. Thus the number of times we can halve n until we get to 1 is $\lceil \lg_2 n \rceil$. Because the recursion goes $\lg n$ levels deep, and a linear amount of work is done per level, mergesort takes $O(n \log n)$ time in the worst case.

Mergesort is a great algorithm for sorting linked lists, because it does not rely on random access to elements as does heapsort or quicksort. Its primary disadvantage is the need for an auxilliary buffer when sorting arrays. It is easy to merge two sorted linked lists without using any extra space, by just rearranging the pointers. However, to merge two sorted arrays (or portions of an array), we need use a third array to store the result of the merge to avoid stepping on the component arrays. Consider merging $\{4, 5, 6\}$ with $\{1, 2, 3\}$, packed from left to right in a single array. Without a buffer, we would overwrite the elements of the top half during merging and lose them.

Mergesort is a classic divide-and-conquer algorithm. We are ahead of the game whenever we can break one large problem into two smaller problems, because the smaller problems are easier to solve. The trick is taking advantage of the two partial solutions to construct a solution of the full problem, as we did with the merge operation.

Implementation

The divide-and-conquer `mergesort` routine follows naturally from the pseudocode:

```
mergesort(item_type s[], int low, int high)
{
        int i;                  /* counter */
        int middle;             /* index of middle element */

        if (low < high) {
                middle = (low+high)/2;
                mergesort(s,low,middle);
                mergesort(s,middle+1,high);
                merge(s, low, middle, high);
        }
}
```

More challenging turns out to be the details of how the merging is done. The problem is that we must put our merged array somewhere. To avoid losing an element by overwriting it in the course of the merge, we first copy each subarray to a separate queue and merge these elements back into the array. In particular:

```
merge(item_type s[], int low, int middle, int high)
{
  int i;                    /* counter */
  queue buffer1, buffer2; /* buffers to hold elements for merging */

  init_queue(&buffer1);
  init_queue(&buffer2);

  for (i=low; i<=middle; i++) enqueue(&buffer1,s[i]);
  for (i=middle+1; i<=high; i++) enqueue(&buffer2,s[i]);

  i = low;
  while (!(empty_queue(&buffer1) || empty_queue(&buffer2))) {
          if (headq(&buffer1) <= headq(&buffer2))
                  s[i++] = dequeue(&buffer1);
          else
                  s[i++] = dequeue(&buffer2);
  }

  while (!empty_queue(&buffer1)) s[i++] = dequeue(&buffer1);
  while (!empty_queue(&buffer2)) s[i++] = dequeue(&buffer2);
}
```

4.6 Quicksort: Sorting by Randomization

Suppose we select a random item p from the n items we seek to sort. *Quicksort* (shown in action in Figure 4.5) separates the $n-1$ other items into two piles: a low pile containing all the elements that appear before p in sorted order and a high pile containing all the elements that appear after p in sorted order. Low and high denote the array positions we place the respective piles, leaving a single slot between them for p.

Such partitioning buys us two things. First, the pivot element p ends up in the exact array position it will reside in the the final sorted order. Second, after partitioning no element flops to the other side in the final sorted order. *Thus we can now sort the elements to the left and the right of the pivot independently!* This gives us a recursive sorting algorithm, since we can use the partitioning approach to sort each subproblem. The algorithm must be correct since each element ultimately ends up in the proper position:

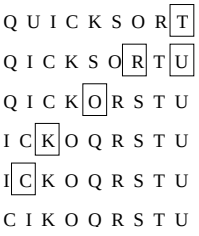

Figure 4.5: Animation of quicksort in action

```
quicksort(item_type s[], int l, int h)
{
        int p;                  /* index of partition */

        if ((h-l)>0) {
                p = partition(s,l,h);
                quicksort(s,l,p-1);
                quicksort(s,p+1,h);
        }
}
```

We can partition the array in one linear scan for a particular pivot element by maintaining three sections of the array: less than the pivot (to the left of `firsthigh`), greater than or equal to the pivot (between `firsthigh` and `i`), and unexplored (to the right of `i`), as implemented below:

```
int partition(item_type s[], int l, int h)
{
        int i;              /* counter */
        int p;              /* pivot element index */
        int firsthigh;      /* divider position for pivot element */

        p = h;
        firsthigh = l;
        for (i=l; i<h; i++)
                if (s[i] < s[p]) {
                        swap(&s[i],&s[firsthigh]);
                        firsthigh ++;
                }
        swap(&s[p],&s[firsthigh]);

        return(firsthigh);
}
```

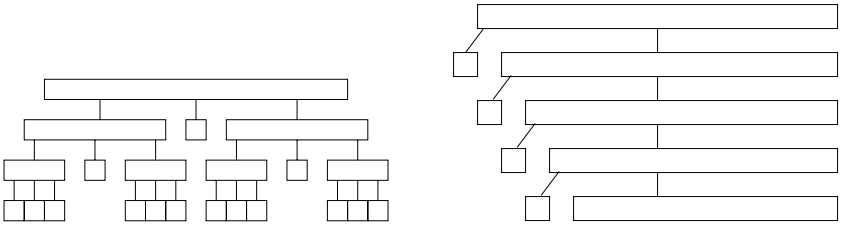

Figure 4.6: The best-case (l) and worst-case (r) recursion trees for quicksort

Since the partitioning step consists of at most n swaps, it takes linear time in the number of keys. But how long does the entire quicksort take? As with mergesort, quicksort builds a recursion tree of nested subranges of the n-element array. As with mergesort, quicksort spends linear time processing (now `partition`ing instead of `merge`ing) the elements in each subarray on each level. As with mergesort, quicksort runs in $O(n \cdot h)$ time, where h is the height of the recursion tree.

The difficulty is that the height of the tree depends upon where the pivot element ends up in each partition. If we get very lucky and *happen* to repeatedly pick the median element as our pivot, the subproblems are always half the size of the previous level. The height represents the number of times we can halve n until we get down to 1, or at most $\lceil \lg_2 n \rceil$. This happy situation is shown in Figure 4.6(l), and corresponds to the best case of quicksort.

Now suppose we consistently get unlucky, and our pivot element always splits the array as unequally as possible. This implies that the pivot element is always the biggest or smallest element in the sub-array. After this pivot settles into its position, we are left with one subproblem of size $n - 1$. We spent linear work and reduced the size of our problem by one measly element, as shown in Figure 4.6(r). It takes a tree of height $n - 1$ to chop our array down to one element per level, for a worst case time of $\Theta(n^2)$.

Thus, the worst case for quicksort is worse than heapsort or mergesort. To justify its name, quicksort had better be good in the average case. Understanding why requires some intuition about random sampling.

4.6.1 Intuition: The Expected Case for Quicksort

The expected performance of quicksort depends upon the height of the partition tree constructed by random pivot elements at each step. Mergesort ran in $O(n \log n)$ time because we split the keys into two equal halves, sorted them recursively, and then merged the halves in linear time. Thus, whenever our pivot element is near the center of the sorted array (i.e. , the pivot is close to the median element), we get a good split and realize the same performance as mergesort.

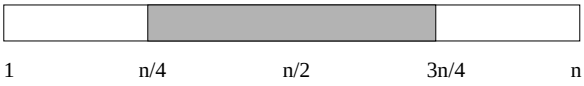

Figure 4.7: Half the time, the pivot is close to the median element

I will give an intuitive explanation of why quicksort is $O(n \log n)$ in the average case. How likely is it that a randomly selected pivot is a good one? The best possible selection for the pivot would be the median key, because exactly half of elements would end up left, and half the elements right, of the pivot. Unfortunately, we only have a probability of $1/n$ of randomly selecting the median as pivot, which is quite small.

Suppose a key is a *good enough* pivot if it lies is in the center half of the sorted space of keys—i.e. , those ranked from $n/4$ to $3n/4$ in the space of all keys to be sorted. Such *good enough* pivot elements are quite plentiful, since half the elements lie closer to the middle than one of the two ends (see Figure 4.7). Thus, on each selection we will pick a *good enough* pivot with probability of $1/2$.

Can you flip a coin so it comes up tails each time? Not without cheating. If you flip a fair coin n times, it will come out heads about half the time. Let heads denote the chance of picking a *good enough* pivot.

The worst possible *good enough* pivot leaves the bigger half of the space partition with $3n/4$ items. What is the height h_g of a quicksort partition tree constructed repeatedly from the worst-possible *good enough* pivot? The deepest path through this tree passes through partitions of size $n, (3/4)n, (3/4)^2 n, \ldots$, down to 1. How many times can we multiply n by $3/4$ until it gets down to 1?

$$(3/4)^{h_g} n = 1 \Rightarrow n = (4/3)^{h_g}$$

so $h_g = \log_{4/3} n$.

But only half of all randomly selected pivots will be *good enough*. The rest we classify as *bad*. The worst of these bad pivots will do essentially nothing to reduce the partition size along the deepest path. The deepest path from the root through a typical randomly-constructed quicksort partition tree will pass through roughly equal numbers of good-enough and bad pivots. Since the expected number of good splits and bad splits is the same, the bad splits can only double the height of the tree, so $h \approx 2h_g = 2 \log_{4/3} n$, which is clearly $\Theta(\log n)$.

On average, random quicksort partition trees (and by analogy, binary search trees under random insertion) are very good. More careful analysis shows the average height after n insertions is approximately $2 \ln n$. Since $2 \ln n \approx 1.386 \lg_2 n$, this is only 39% taller than a perfectly balanced binary tree. Since quicksort does $O(n)$ work partitioning on each level, the average time is $O(n \log n)$. If we are *extremely* unlucky and our randomly selected elements always are among the largest or smallest element in the array, quicksort turns into selection sort and runs in $O(n^2)$. However, the odds against this are vanishingly small.

4.6.2 Randomized Algorithms

There is an important subtlety about the expected case $O(n \log n)$ running time for quicksort. Our quicksort implementation above selected the last element in each sub-array as the pivot. Suppose this program were given a sorted array as input. If so, at each step it would pick the worst possible pivot and run in quadratic time.

For any deterministic method of pivot selection, there exists a worst-case input instance which will doom us to quadratic time. The analysis presented above made no claim stronger than:

> "Quicksort runs in $\Theta(n \log n)$ time, with high probability, *if* you give me randomly ordered data to sort."

But now suppose we add an initial step to our algorithm where we randomly permute the order of the n elements before we try to sort them. Such a permutation can be constructed in $O(n)$ time (see Section 13.7 for details). This might seem like wasted effort, but it provides the guarantee that we can expect $\Theta(n \log n)$ running time *whatever* the initial input was. The worst case performance still can happen, but it depends only upon how unlucky we are. There is no longer a well-defined "worst case" input. We now can say

> "Randomized quicksort runs in $\Theta(n \log n)$ time on *any* input, with high probability."

Alternately, we could get the same guarantee by selecting a random element to be the pivot at each step.

Randomization is a powerful tool to improve algorithms with bad worst-case but good average-case complexity. It can be used to make algorithms more robust to boundary cases and more efficient on highly structured input instances that confound heuristic decisions (such as sorted input to quicksort). It often lends itself to simple algorithms that provide randomized performance guarantees which are otherwise obtainable only using complicated deterministic algorithms.

Proper analysis of randomized algorithms requires some knowledge of probability theory, and is beyond the scope of this book. However, some of the approaches to designing efficient randomized algorithms are readily explainable:

- *Random sampling* – Want to get an idea of the median value of n things but don't have either the time or space to look at them all? Select a small random sample of the input and study those, for the results should be representative.

  This is the idea behind opinion polling. Biases creep in unless you take a truly *random* sample, as opposed to the first x people you happen to see. To avoid bias, actual polling agencies typically dial random phone numbers and hope someone answers.

- *Randomized hashing* – We have claimed that hashing can be used to implement dictionary operations in $O(1)$ "expected-time." However, for any hash

function there is a given worst-case set of keys that all get hashed to the same bucket. But now suppose we randomly select our hash function from a large family of good ones as the first step of our algorithm. We get the same type of improved guarantee that we did with randomized quicksort.

- *Randomized search* – Randomization can also be used to drive search techniques such as simulated annealing, as will be discussed in detail in Section 7.5.3 (page 254).

Stop and Think: Nuts and Bolts

Problem: The *nuts and bolts* problem is defined as follows. You are given a collection of n bolts of different widths, and n corresponding nuts. You can test whether a given nut and bolt fit together, from which you learn whether the nut is too large, too small, or an exact match for the bolt. The differences in size between pairs of nuts or bolts are too small to see by eye, so you cannot compare the sizes of two nuts or two bolts directly. You are to match each bolt to each nut.

Give an $O(n^2)$ algorithm to solve the nuts and bolts problem. Then give a randomized $O(n \log n)$ expected time algorithm for the same problem.

Solution: The brute force algorithm for matching nuts and bolts starts with the first bolt and compares it to each nut until we find a match. In the worst case, this will require n comparisons. Repeating this for each successive bolt on all remaining nuts yields a quadratic-comparison algorithm.

What if we pick a random bolt and try it? On average, we would expect to get about halfway through the set of nuts before we found the match, so this randomized algorithm would do half the work as the worst case. That counts as some kind of improvement, although not an asymptotic one.

Randomized quicksort achieves the desired expected-case running time, so a natural idea is to emulate it on the nuts and bolts problem. Indeed, sorting both the nuts and bolts by size would yield a matching, since the ith largest nut must match the ith largest bolt.

The fundamental step in quicksort is partitioning elements around a pivot. Can we partition nuts and bolts around a randomly selected bolt b? Certainly we can partition the nuts into those of size less than b and greater than b. But decomposing the problem into two halves requires partitioning the bolts as well, and we cannot compare bolt against bolt. But once we find the matching nut to b we can use it to partition the bolts accordingly. In $2n - 2$ comparisons, we partition the nuts and bolts, and the remaining analysis follows directly from randomized quicksort.

What is interesting about this problem is that no simple deterministic algorithm for nut and bolt sorting is known. It illustrates how randomization makes the bad case go away, leaving behind a simple and beautiful algorithm. ∎

4.6.3 Is Quicksort Really Quick?

There is a clear, asymptotic difference between an $\Theta(n \log n)$ algorithm and one that runs in $\Theta(n^2)$. Thus, only the most obstinate reader would doubt my claim that mergesort, heapsort, and quicksort should all outperform insertion sort or selection sort on large enough instances.

But how can we compare two $\Theta(n \log n)$ algorithms to decide which is faster? How can we prove that quicksort is really quick? Unfortunately, the RAM model and Big Oh analysis provide too coarse a set of tools to make that type of distinction. When faced with algorithms of the same asymptotic complexity, implementation details and system quirks such as cache performance and memory size may well prove to be the decisive factor.

What we can say is that experiments show that where a properly implemented quicksort is implemented well, it is typically 2-3 times faster than mergesort or heapsort. The primary reason is that the operations in the innermost loop are simpler. But I can't argue with you if you don't believe me when I say quicksort is faster. It is a question whose solution lies outside the analytical tools we are using. The best way to tell is to implement both algorithms and experiment.

4.7 Distribution Sort: Sorting via Bucketing

We could sort sorting names for the telephone book by partitioning them according to the first letter of the last name. This will create 26 different piles, or buckets, of names. Observe that any name in the J pile must occur after every name in the I pile, but before any name in the K pile. Therefore, we can proceed to sort each pile individually and just concatenate the bunch of sorted piles together at the end.

If the names are distributed evenly among the buckets, the resulting 26 sorting problems should each be substantially smaller than the original problem. Further, by now partitioning each pile based on the second letter of each name, we generate smaller and smaller piles. The names will be sorted as soon as each bucket contains only a single name. The resulting algorithm is commonly called *bucketsort* or *distribution sort*.

Bucketing is a very effective idea whenever we are confident that the distribution of data will be roughly uniform. It is the idea that underlies hash tables, *kd*-trees, and a variety of other practical data structures. The downside of such techniques is that the performance can be terrible when the data distribution is not what we expected. Although data structures such as balanced binary trees offer guaranteed worst-case behavior for any input distribution, no such promise exists for heuristic data structures on unexpected input distributions.

Nonuniform distributions do occur in real life. Consider Americans with the uncommon last name of Shifflett. When last I looked, the Manhattan telephone directory (with over one million names) contained exactly five Shiffletts. So how many Shiffletts should there be in a small city of 50,000 people? Figure 4.8 shows

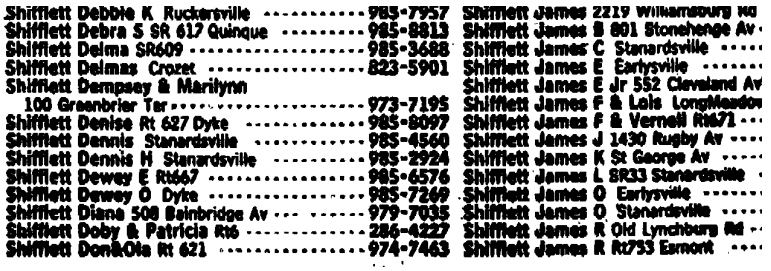

Figure 4.8: A small subset of Charlottesville Shiffletts

a small portion of the *two and a half pages* of Shiffletts in the Charlottesville, Virginia telephone book. The Shifflett clan is a fixture of the region, but it would play havoc with any distribution sort program, as refining buckets from S to Sh to Shi to $Shif$ to ... to $Shifflett$ results in no significant partitioning.

Take-Home Lesson: Sorting can be used to illustrate most algorithm design paradigms. Data structure techniques, divide-and-conquer, randomization, and incremental construction all lead to efficient sorting algorithms.

4.7.1 Lower Bounds for Sorting

One last issue on the complexity of sorting. We have seen several sorting algorithms that run in worst-case $O(n \log n)$ time, but none of which is linear. To sort n items certainly requires looking at all of them, so any sorting algorithm must be $\Omega(n)$ in the worst case. Can we close this remaining $\Theta(\log n)$ gap?

The answer is no. An $\Omega(n \log n)$ lower bound can be shown by observing that any sorting algorithm must behave differently during execution on each of the distinct $n!$ permutations of n keys. The outcome of each pairwise comparison governs the run-time behavior of any comparison-based sorting algorithm. We can think of the set of all possible executions of such an algorithm as a tree with $n!$ leaves. The minimum height tree corresponds to the fastest possible algorithm, and it happens that $\lg(n!) = \Theta(n \log n)$.

This lower bound is important for several reasons. First, the idea can be extended to give lower bounds for many applications of sorting, including element uniqueness, finding the mode, and constructing convex hulls. Sorting has one of the few nontrivial lower bounds among algorithmic problems. We will present an alternate approach to arguing that fast algorithms are unlikely to exist in Chapter 9.

4.8 War Story: Skiena for the Defense

I lead a quiet, reasonably honest life. One reward for this is that I don't often find myself on the business end of surprise calls from lawyers. Thus I was astonished to get a call from a lawyer who not only wanted to talk with me, but wanted to talk to me about sorting algorithms.

It turned out that her firm was working on a case involving high-performance programs for sorting, and needed an expert witness who could explain technical issues to the jury. From the first edition of this book, they could see I knew something about algorithms, but before taking me on they demanded to see my teaching evaluations to prove that I could explain things to people.[2] It proved to be a fascinating opportunity to learn about how *really* fast sorting programs work. I figured I could finally answer the question of which in-place sorting algorithm was fastest in practice. Was it heapsort or quicksort? What subtle, secret algorithmics made the difference to minimize the number of comparisons in practice?

The answer was quite humbling. *Nobody cared about in-place sorting.* The name of the game was sorting *huge* files, much bigger than could fit in main memory. All the important action was in getting the the data on and off a disk. Cute algorithms for doing internal (in-memory) sorting were not particularly important because the real problem lies in sorting gigabytes at a time.

Recall that disks have relatively long seek times, reflecting how long it takes the desired part of the disk to rotate under the read/write head. Once the head is in the right place, the data moves relatively quickly, and it costs about the same to read a large data block as it does to read a single byte. Thus, the goal is minimizing the number of blocks read/written, and coordinating these operations so the sorting algorithm is never waiting to get the data it needs.

The disk-intensive nature of sorting is best revealed by the annual *Minutesort* competition. The goal is to sort as much data in one minute as possible. The current champion is Jim Wyllie of IBM Research, who managed to sort 116 gigabytes of data in 58.7 seconds on his little old 40-node 80-Itanium cluster with a SAN array of 2,520 disks. Slightly more down-to-earth is the *Pennysort* division, where the goal is the maximized sorting performance per penny of hardware. The current champ here (*BSIS* from China) sorted 32 gigabytes in 1,679 seconds on a $760 PC containing four SATA drives. You can check out the current records at *http://research.microsoft.com/barc/SortBenchmark/*.

That said, which algorithm is best for external sorting? It basically turns out to be a multiway mergesort, employing a lot of engineering and special tricks. You build a heap with members of the top block from each of k sorted lists. By repeatedly plucking the top element off this heap, you build a sorted list merging these k lists. Because this heap is sitting in main memory, these operations are fast. When you have a large enough sorted run, you write it to disk and free up

[2] One of my more cynical faculty colleagues said this was the first time anyone, anywhere, had ever looked at university teaching evaluations.

memory for more data. Once you start to run out of elements from the top block of one of the k sorted lists you are merging, load the next block.

It proves very hard to benchmark sorting programs/algorithms at this level and decide which is *really* fastest. Is it fair to compare a commercial program designed to handle general files with a stripped-down code optimized for integers? The *Minutesort* competition employs randomly-generated 100-byte records. This is a different world than sorting names or integers. For example, one widely employed trick is to strip off a relatively short prefix of the key and initially sort just on that, to avoid lugging around all those extra bytes.

What lessons can be learned from this? The most important, by far, is to do everything you can to avoid being involved in a lawsuit as either a plaintiff or defendant.[3] Courts are not instruments for resolving disputes quickly. Legal battles have a lot in common with military battles: they escalate very quickly, become very expensive in time, money, and soul, and usually end only when both sides are exhausted and compromise. Wise are the parties who can work out their problems without going to court. Properly absorbing this lesson now could save you thousands of times the cost of this book.

On technical matters, it is important to worry about external memory performance whenever you combine very large datasets with low-complexity algorithms (say linear or $n \log n$). Constant factors of even 5 or 10 can make a big difference then between what is feasible and what is hopeless. Of course, quadratic-time algorithms are doomed to fail on large datasets regardless of data access times.

4.9 Binary Search and Related Algorithms

Binary search is a fast algorithm for searching in a sorted array of keys S. To search for key q, we compare q to the middle key $S[n/2]$. If q appears before $S[n/2]$, it must reside in the top half of S; if not, it must reside in the bottom half of S. By repeating this process recursively on the correct half, we locate the key in a total of $\lceil \lg n \rceil$ comparisons—a big win over the $n/2$ comparisons expect using sequential search:

```
int binary_search(item_type s[], item_type key, int low, int high)
{
      int middle;                    /* index of middle element */

      if (low > high) return (-1);  /* key not found */

      middle = (low+high)/2;
```

[3]It is actually quite interesting serving as an expert witness.

```
        if (s[middle] == key) return(middle);

        if (s[middle] > key)
                return( binary_search(s,key,low,middle-1) );
        else
                return(binary_search(s,key,middle+1,high) );
}
```

This much you probably know. What is important is to have a sense of just how fast binary search is. *Twenty questions* is a popular children's game where one player selects a word and the other repeatedly asks true/false questions in an attempt to guess it. If the word remains unidentified after 20 questions, the first party wins; otherwise, the second player takes the honors. In fact, the second player always has a winning strategy, based on binary search. Given a printed dictionary, the player opens it in the middle, selects a word (say "move"), and asks whether the unknown word is before "move" in alphabetical order. Since standard dictionaries contain 50,000 to 200,000 words, we can be certain that the process will terminate within twenty questions.

4.9.1 Counting Occurrences

Several interesting algorithms follow from simple variants of binary search. Suppose that we want to count the number of times a given key k (say "Skiena") occurs in a given sorted array. Because sorting groups all the copies of k into a contiguous block, the problem reduces to finding the right block and then measures its size.

The binary search routine presented above enables us to find the index of an element of the correct block (x) in $O(\lg n)$ time. The natural way to identify the boundaries of the block is to sequentially test elements to the left of x until we find the first one that differs from the search key, and then repeat this search to the right of x. The difference between the indices of the left and right boundaries (plus one) gives the count of the number of occurrences of k.

This algorithm runs in $O(\lg n + s)$, where s is the number of occurrences of the key. This can be as bad as linear if the entire array consists of identical keys. A faster algorithm results by modifying binary search to search for the *boundary* of the block containing k, instead of k itself. Suppose we delete the equality test

```
if (s[middle] == key) return(middle);
```

from the implementation above and return the index `low` instead of -1 on each unsuccessful search. *All* searches will now be unsuccessful, since there is no equality test. The search will proceed to the right half whenever the key is compared to an identical array element, eventually terminating at the right boundary. Repeating the search after reversing the direction of the binary comparison will lead us to the left boundary. Each search takes $O(\lg n)$ time, so we can count the occurrences in logarithmic time regardless of the size of the block.

4.9.2 One-Sided Binary Search

Now suppose we have an array A consisting of a run of 0's, followed by an unbounded run of 1's, and would like to identify the exact point of transition between them. Binary search on the array would provide the transition point in $\lceil \lg n \rceil$ tests, if we had a bound n on the number of elements in the array. In the absence of such a bound, we can test repeatedly at larger intervals ($A[1]$, $A[2]$, $A[4]$, $A[8]$, $A[16]$, ...) until we find a first nonzero value. Now we have a window containing the target and can proceed with binary search. This *one-sided binary search* finds the transition point p using at most $2\lceil \lg p \rceil$ comparisons, regardless of how large the array actually is. One-sided binary search is most useful whenever we are looking for a key that lies close to our current position.

4.9.3 Square and Other Roots

The square root of n is the number r such that $r^2 = n$. Square root computations are performed inside every pocket calculator, but it is instructive to develop an efficient algorithm to compute them.

First, observe that the square root of $n \geq 1$ must be at least 1 and at most n. Let $l = 1$ and $r = n$. Consider the midpoint of this interval, $m = (l + r)/2$. How does m^2 compare to n? If $n \geq m^2$, then the square root must be greater than m, so the algorithm repeats with $l = m$. If $n < m^2$, then the square root must be less than m, so the algorithm repeats with $r = m$. Either way, we have halved the interval using only one comparison. Therefore, after $\lg n$ rounds we will have identified the square root to within ± 1.

This bisection method, as it is called in numerical analysis, can also be applied to the more general problem of finding the roots of an equation. We say that x is a *root* of the function f if $f(x) = 0$. Suppose that we start with values l and r such that $f(l) > 0$ and $f(r) < 0$. If f is a continuous function, there must exist a root between l and r. Depending upon the sign of $f(m)$, where $m = (l + r)/2$, we can cut this window containing the root in half with each test and stop soon as our estimate becomes sufficiently accurate.

Root-finding algorithms that converge faster than binary search are known for both of these problems. Instead of always testing the midpoint of the interval, these algorithms interpolate to find a test point closer to the actual root. Still, binary search is simple, robust, and works as well as possible without additional information on the nature of the function to be computed.

Take-Home Lesson: Binary search and its variants are the quintessential divide-and-conquer algorithms.

4.10 Divide-and-Conquer

One of the most powerful techniques for solving problems is to break them down into smaller, more easily solved pieces. Smaller problems are less overwhelming, and they permit us to focus on details that are lost when we are studying the entire problem. A recursive algorithm starts to become apparent when we can break the problem into smaller instances of the same type of problem. Effective parallel processing requires decomposing jobs into at least as many tasks as processors, and is becoming more important with the advent of cluster computing and multicore processors.

Two important algorithm design paradigms are based on breaking problems down into smaller problems. In Chapter 8, we will see dynamic programming, which typically removes one element from the problem, solves the smaller problem, and then uses the solution to this smaller problem to add back the element in the proper way. *Divide-and-conquer* instead splits the problem in (say) halves, solves each half, then stitches the pieces back together to form a full solution.

To use divide-and-conquer as an algorithm design technique, we must divide the problem into two smaller subproblems, solve each of them recursively, and then meld the two partial solutions into one solution to the full problem. Whenever the merging takes less time than solving the two subproblems, we get an efficient algorithm. Mergesort, discussed in Section 4.5 (page 120), is the classic example of a divide-and-conquer algorithm. It takes only linear time to merge two sorted lists of $n/2$ elements, each of which was obtained in $O(n \lg n)$ time.

Divide-and-conquer is a design technique with many important algorithms to its credit, including mergesort, the fast Fourier transform, and Strassen's matrix multiplication algorithm. Beyond binary search and its many variants, however, I find it to be a difficult design technique to apply in practice. Our ability to analyze divide-and-conquer algorithms rests on our strength to solve the asymptotics of recurrence relations governing the cost of such recursive algorithms.

4.10.1 Recurrence Relations

Many divide-and-conquer algorithms have time complexities that are naturally modeled by recurrence relations. Evaluating such recurrences is important to understanding when divide-and-conquer algorithms perform well, and provide an important tool for analysis in general. The reader who balks at the very idea of analysis is free to skip this section, but there are important insights into design that come from an understanding of the behavior of recurrence relations.

What is a recurrence relation? It is an equation that is defined in terms of itself. The Fibonacci numbers are described by the recurrence relation $F_n = F_{n-1} + F_{n-2}$ and discussed in Section 8.1.1. Many other natural functions are easily expressed as recurrences. Any polynomial can be represented by a recurrence, such as the linear function:

$$a_n = a_{n-1} + 1, a_1 = 1 \longrightarrow a_n = n$$

Any exponential can be represented by a recurrence:

$$a_n = 2a_{n-1}, a_1 = 1 \longrightarrow a_n = 2^{n-1}$$

Finally, lots of weird functions that cannot be described easily with conventional notation can be represented by a recurrence:

$$a_n = na_{n-1}, a_1 = 1 \longrightarrow a_n = n!$$

This means that recurrence relations are a very versatile way to represent functions.

The self-reference property of recurrence relations is shared with recursive programs or algorithms, as the shared roots of both terms reflect. Essentially, recurrence relations provide a way to analyze recursive structures, such as algorithms.

4.10.2 Divide-and-Conquer Recurrences

Divide-and-conquer algorithms tend to break a given problem into some number of smaller pieces (say a), each of which is of size n/b. Further, they spend $f(n)$ time to combine these subproblem solutions into a complete result. Let $T(n)$ denote the worst-case time the algorithm takes to solve a problem of size n. Then $T(n)$ is given by the following recurrence relation:

$$T(n) = aT(n/b) + f(n)$$

Consider the following examples:

- *Sorting* – The running time behavior of mergesort is governed by the recurrence $T(n) = 2T(n/2) + O(n)$, since the algorithm divides the data into equal-sized halves and then spends linear time merging the halves after they are sorted. In fact, this recurrence evaluates to $T(n) = O(n \lg n)$, just as we got by our previous analysis.

- *Binary Search* – The running time behavior of binary search is governed by the recurrence $T(n) = T(n/2) + O(1)$, since at each step we spend constant time to reduce the problem to an instance half its size. In fact, this recurrence evaluates to $T(n) = O(\lg n)$, just as we got by our previous analysis.

- *Fast Heap Construction* – The `bubble_down` method of heap construction (described in Section 4.3.4) built an n-element heap by constructing two $n/2$ element heaps and then merging them with the root in logarithmic time. This argument reduces to the recurrence relation $T(n) = 2T(n/2) + O(\lg n)$. In fact, this recurrence evaluates to $T(n) = O(n)$, just as we got by our previous analysis.

- *Matrix Multiplication* – As discussed in Section 2.5.4, the standard matrix multiplication algorithm for two $n \times n$ matrices takes $O(n^3)$, because we compute the dot product of n terms for each of the n^2 elements in the product matrix.

However, Strassen [Str69] discovered a divide-and-conquer algorithm that manipulates the products of seven $n/2 \times n/2$ matrix products to yield the product of two $n \times n$ matrices. This yields a time-complexity recurrence $T(n) = 7T(n/2) + O(n^2)$. In fact, this recurrence evaluates to $T(n) = O(n^{2.81})$, which seems impossible to predict *without* solving the recurrence.

4.10.3 Solving Divide-and-Conquer Recurrences (*)

In fact, divide-and-conquer recurrences of the form $T(n) = aT(n/b) + f(n)$ are generally easy to solve, because the solutions typically fall into one of three distinct cases:

1. If $f(n) = O(n^{\log_b a - \epsilon})$ for some constant $\epsilon > 0$, then $T(n) = \Theta(n^{\log_b a})$.
2. If $f(n) = \Theta(n^{\log_b a})$, then $T(n) = \Theta(n^{\log_b a} \lg n)$.
3. If $f(n) = \Omega(n^{\log_b a + \epsilon})$ for some constant $\epsilon > 0$, and if $af(n/b) \leq cf(n)$ for some $c < 1$, then $T(n) = \Theta(f(n))$.

Although this looks somewhat frightening, it really isn't difficult to apply. The issue is identifying which case of the so-called *master theorem* holds for your given recurrence. Case 1 holds for heap construction and matrix multiplication, while Case 2 holds mergesort and binary search. Case 3 generally arises for clumsier algorithms, where the cost of combining the subproblems dominates everything.

The master theorem can be thought of as a black-box piece of machinery, invoked as needed and left with its mystery intact. However, with a little study, the reason why the master theorem works can become apparent.

Figure 4.9 shows the recursion tree associated with a typical $T(n) = aT(n/b) + f(n)$ divide-and-conquer algorithm. Each problem of size n is decomposed into a problems of size n/b. Each subproblem of size k takes $O(f(k))$ time to deal with internally, between partitioning and merging. The total time for the algorithm is the sum of these internal costs, plus the overhead of building the recursion tree. The height of this tree is $h = \log_b n$ and the number of leaf nodes $a^h = a^{\log_b n}$, which happens to simplify to $n^{\log_b a}$ with some algebraic manipulation.

The three cases of the master theorem correspond to three different costs which might be dominant as a function of a, b, and $f(n)$:

- *Case 1: Too many leaves* – If the number of leaf nodes outweighs the sum of the internal evaluation cost, the total running time is $O(n^{\log_b a})$.
- *Case 2: Equal work per level* – As we move down the tree, each problem gets smaller but there are more of them to solve. If the sum of the internal evaluation costs at each level are equal, the total running time is the cost per level ($n^{\log_b a}$) times the number of levels ($\log_b n$), for a total running time of $O(n^{\log_b a} \lg n)$.

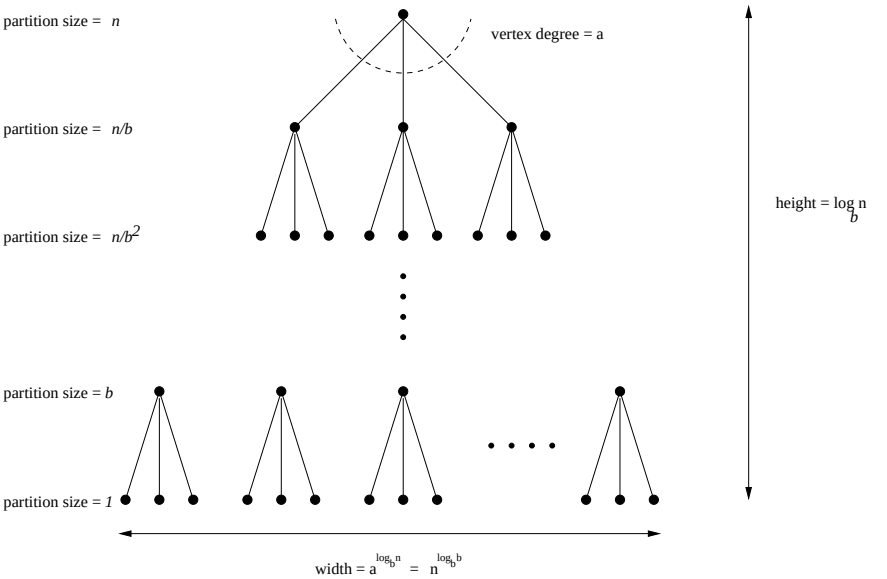

Figure 4.9: The recursion tree resulting from decomposing each problem of size n into a problems of size n/b

- *Case 3: Too expensive a root* – If the internal evaluation costs grow rapidly enough with n, then the cost of the root evaluation may dominate. If so, the the total running time is $O(f(n))$.

Chapter Notes

The most interesting sorting algorithms that have not been discussed in this section include *shellsort*, which is a substantially more efficient version of insertion sort, and *radix sort*, an efficient algorithm for sorting strings. You can learn more about these and every other sorting algorithm by browsing through Knuth [Knu98], with hundreds of pages of interesting material on sorting. This includes external sorting, the subject of this chapter's legal war story.

As implemented here, mergesort copies the merged elements into an auxiliary buffer to avoid overwriting the original elements to be sorted. Through clever but complicated buffer manipulation, mergesort can be implemented in an array without using much extra storage. Kronrod's algorithm for in-place merging is presented in [Knu98].

Randomized algorithms are discussed in greater detail in the books by Motwani and Raghavan [MR95] and Mitzenmacher and Upfal [MU05]. The problem of

nut and bolt sorting was introduced by [Raw92]. A complicated but deterministic $O(n \log n)$ algorithm is due to Komlos, Ma, and Szemeredi [KMS96].

Several other algorithms texts provide more substantive coverage of divide-and-conquer algorithms, including [CLRS01, KT06, Man89]. See [CLRS01] for an excellent overview of the master theorem.

4.11 Exercises

Applications of Sorting

4-1. *[3]* The Grinch is given the job of partitioning $2n$ players into two teams of n players each. Each player has a numerical rating that measures how good he/she is at the game. He seeks to divide the players as *unfairly* as possible, so as to create the biggest possible talent imbalance between team A and team B. Show how the Grinch can do the job in $O(n \log n)$ time.

4-2. *[3]* For each of the following problems, give an algorithm that finds the desired numbers within the given amount of time. To keep your answers brief, feel free to use algorithms from the book as subroutines. For the example, $S = \{6, 13, 19, 3, 8\}$, $19 - 3$ maximizes the difference, while $8 - 6$ minimizes the difference.

(a) Let S be an *unsorted* array of n integers. Give an algorithm that finds the pair $x, y \in S$ that *maximizes* $|x - y|$. Your algorithm must run in $O(n)$ worst-case time.

(b) Let S be a *sorted* array of n integers. Give an algorithm that finds the pair $x, y \in S$ that *maximizes* $|x - y|$. Your algorithm must run in $O(1)$ worst-case time.

(c) Let S be an *unsorted* array of n integers. Give an algorithm that finds the pair $x, y \in S$ that *minimizes* $|x - y|$, for $x \neq y$. Your algorithm must run in $O(n \log n)$ worst-case time.

(d) Let S be a *sorted* array of n integers. Give an algorithm that finds the pair $x, y \in S$ that *minimizes* $|x - y|$, for $x \neq y$. Your algorithm must run in $O(n)$ worst-case time.

4-3. *[3]* Take a sequence of $2n$ real numbers as input. Design an $O(n \log n)$ algorithm that partitions the numbers into n pairs, with the property that the partition minimizes the maximum sum of a pair. For example, say we are given the numbers (1,3,5,9). The possible partitions are ((1,3),(5,9)), ((1,5),(3,9)), and ((1,9),(3,5)). The pair sums for these partitions are (4,14), (6,12), and (10,8). Thus the third partition has 10 as its maximum sum, which is the minimum over the three partitions.

4-4. *[3]* Assume that we are given n pairs of items as input, where the first item is a number and the second item is one of three colors (red, blue, or yellow). Further assume that the items are sorted by number. Give an $O(n)$ algorithm to sort the items by color (all reds before all blues before all yellows) such that the numbers for identical colors stay sorted.

For example: (1,blue), (3,red), (4,blue), (6,yellow), (9,red) should become (3,red), (9,red), (1,blue), (4,blue), (6,yellow).

4-5. *[3]* The *mode* of a set of numbers is the number that occurs most frequently in the set. The set $(4, 6, 2, 4, 3, 1)$ has a mode of 4. Give an efficient and correct algorithm to compute the mode of a set of n numbers.

4-6. *[3]* Given two sets S_1 and S_2 (each of size n), and a number x, describe an $O(n \log n)$ algorithm for finding whether there exists a pair of elements, one from S_1 and one from S_2, that add up to x. (For partial credit, give a $\Theta(n^2)$ algorithm for this problem.)

4-7. *[3]* Outline a reasonable method of solving each of the following problems. Give the order of the worst-case complexity of your methods.

(a) You are given a pile of thousands of telephone bills and thousands of checks sent in to pay the bills. Find out who did not pay.

(b) You are given a list containing the title, author, call number and publisher of all the books in a school library and another list of 30 publishers. Find out how many of the books in the library were published by each company.

(c) You are given all the book checkout cards used in the campus library during the past year, each of which contains the name of the person who took out the book. Determine how many distinct people checked out at least one book.

4-8. *[4]* Given a set of S containing n real numbers, and a real number x. We seek an algorithm to determine whether two elements of S exist whose sum is exactly x.

(a) Assume that S is unsorted. Give an $O(n \log n)$ algorithm for the problem.

(b) Assume that S is sorted. Give an $O(n)$ algorithm for the problem.

4-9. *[4]* Give an efficient algorithm to compute the union of sets A and B, where $n = \max(|A|, |B|)$. The output should be an array of distinct elements that form the union of the sets, such that they appear more than once in the union.

(a) Assume that A and B are unsorted. Give an $O(n \log n)$ algorithm for the problem.

(b) Assume that A and B are sorted. Give an $O(n)$ algorithm for the problem.

4-10. *[5]* Given a set S of n integers and an integer T, give an $O(n^{k-1} \log n)$ algorithm to test whether k of the integers in S add up to T.

4-11. *[6]* Design an $O(n)$ algorithm that, given a list of n elements, finds all the elements that appear more than $n/2$ times in the list. *Then*, design an $O(n)$ algorithm that, given a list of n elements, finds all the elements that appear more than $n/4$ times.

Heaps

4-12. *[3]* Devise an algorithm for finding the k smallest elements of an unsorted set of n integers in $O(n + k \log n)$.

4-13. *[5]* You wish to store a set of n numbers in either a max-heap or a sorted array. For each application below, state which data structure is better, or if it does not matter. Explain your answers.

(a) Want to find the maximum element quickly.

(b) Want to be able to delete an element quickly.

(c) Want to be able to form the structure quickly.

(d) Want to find the minimum element quickly.

4-14. *[5]* Give an $O(n \log k)$-time algorithm that merges k sorted lists with a total of n elements into one sorted list. (Hint: use a heap to speed up the elementary $O(kn)$-time algorithm).

4-15. *[5]* (a) Give an efficient algorithm to find the second-largest key among n keys. You can do better than $2n - 3$ comparisons.

(b) Then, give an efficient algorithm to find the third-largest key among n keys. How many key comparisons does your algorithm do in the worst case? Must your algorithm determine which key is largest and second-largest in the process?

Quicksort

4-16. *[3]* Use the partitioning idea of quicksort to give an algorithm that finds the *median* element of an array of n integers in expected $O(n)$ time. (Hint: must you look at both sides of the partition?)

4-17. *[3]* The *median* of a set of n values is the $\lceil n/2 \rceil$th smallest value.

(a) Suppose quicksort always pivoted on the median of the current sub-array. How many comparisons would Quicksort make then in the worst case?

(b) Suppose quicksort were always to pivot on the $\lceil n/3 \rceil$th smallest value of the current sub-array. How many comparisons would be made then in the worst case?

4-18. *[5]* Suppose an array A consists of n elements, each of which is *red*, *white*, or *blue*. We seek to sort the elements so that all the *reds* come before all the *whites*, which come before all the *blues* The only operation permitted on the keys are

- *Examine(A,i)* – report the color of the ith element of A.
- *Swap(A,i,j)* – swap the ith element of A with the jth element.

Find a correct and efficient algorithm for red-white-blue sorting. There is a linear-time solution.

4-19. *[5]* An *inversion* of a permutation is a pair of elements that are out of order.

(a) Show that a permutation of n items has at most $n(n-1)/2$ inversions. Which permutation(s) have exactly $n(n-1)/2$ inversions?

(b) Let P be a permutation and P^r be the reversal of this permutation. Show that P and P^r have a total of exactly $n(n-1)/2$ inversions.

(c) Use the previous result to argue that the expected number of inversions in a random permutation is $n(n-1)/4$.

4-20. *[3]* Give an efficient algorithm to rearrange an array of n keys so that all the negative keys precede all the nonnegative keys. Your algorithm must be in-place, meaning you cannot allocate another array to temporarily hold the items. How fast is your algorithm?

Other Sorting Algorithms

4-21. *[5]* Stable sorting algorithms leave equal-key items in the same relative order as in the original permutation. Explain what must be done to ensure that mergesort is a stable sorting algorithm.

4-22. *[3]* Show that n positive integers in the range 1 to k can be sorted in $O(n \log k)$ time. The interesting case is when $k << n$.

4-23. *[5]* We seek to sort a sequence S of n integers with many duplications, such that the number of distinct integers in S is $O(\log n)$. Give an $O(n \log \log n)$ worst-case time algorithm to sort such sequences.

4-24. *[5]* Let $A[1..n]$ be an array such that the first $n - \sqrt{n}$ elements are already sorted (though we know nothing about the remaining elements). Give an algorithm that sorts A in substantially better than $n \log n$ steps.

4-25. *[5]* Assume that the array $A[1..n]$ only has numbers from $\{1, \ldots, n^2\}$ but that at most $\log \log n$ of these numbers ever appear. Devise an algorithm that sorts A in substantially less than $O(n \log n)$.

4-26. *[5]* Consider the problem of sorting a sequence of n 0's and 1's using comparisons. For each comparison of two values x and y, the algorithm learns which of $x < y$, $x = y$, or $x > y$ holds.

(a) Give an algorithm to sort in $n - 1$ comparisons in the worst case. Show that your algorithm is optimal.

(b) Give an algorithm to sort in $2n/3$ comparisons in the average case (assuming each of the n inputs is 0 or 1 with equal probability). Show that your algorithm is optimal.

4-27. *[6]* Let P be a simple, but not necessarily convex, polygon and q an arbitrary point not necessarily in P. Design an efficient algorithm to find a line segment originating from q that intersects the maximum number of edges of P. In other words, if standing at point q, in what direction should you aim a gun so the bullet will go through the largest number of walls. A bullet through a vertex of P gets credit for only one wall. An $O(n \log n)$ algorithm is possible.

Lower Bounds

4-28. *[5]* In one of my research papers [Ski88], I discovered a comparison-based sorting algorithm that runs in $O(n \log(\sqrt{n}))$. Given the existence of an $\Omega(n \log n)$ lower bound for sorting, how can this be possible?

4-29. *[5]* Mr. B. C. Dull claims to have developed a new data structure for priority queues that supports the operations *Insert*, *Maximum*, and *Extract-Max*—all in $O(1)$ worst-case time. Prove that he is mistaken. (Hint: the argument does not involve a lot of gory details—just think about what this would imply about the $\Omega(n \log n)$ lower bound for sorting.)

Searching

4-30. *[3]* A company database consists of 10,000 sorted names, 40% of whom are known as good customers and who together account for 60% of the accesses to the database. There are two data structure options to consider for representing the database:

- Put all the names in a single array and use binary search.
- Put the good customers in one array and the rest of them in a second array. Only if we do not find the query name on a binary search of the first array do we do a binary search of the second array.

Demonstrate which option gives better expected performance. Does this change if linear search on an unsorted array is used instead of binary search for both options?

4-31. *[3]* Suppose you are given an array A of n sorted numbers that has been *circularly shifted* k positions to the right. For example, $\{35, 42, 5, 15, 27, 29\}$ is a sorted array that has been circularly shifted $k = 2$ positions, while $\{27, 29, 35, 42, 5, 15\}$ has been shifted $k = 4$ positions.

- Suppose you know what k is. Give an $O(1)$ algorithm to find the largest number in A.
- Suppose you *do not* know what k is. Give an $O(\lg n)$ algorithm to find the largest number in A. For partial credit, you may give an $O(n)$ algorithm.

4-32. *[3]* Consider the numerical 20 Questions game. In this game, Player 1 thinks of a number in the range 1 to n. Player 2 has to figure out this number by asking the fewest number of true/false questions. Assume that nobody cheats.

(a) What is an optimal strategy if n in known?

(b) What is a good strategy is n is not known?

4-33. *[5]* Suppose that you are given a sorted sequence of *distinct* integers $\{a_1, a_2, \ldots, a_n\}$. Give an $O(\lg n)$ algorithm to determine whether there exists an i index such as $a_i = i$. For example, in $\{-10, -3, 3, 5, 7\}$, $a_3 = 3$. In $\{2, 3, 4, 5, 6, 7\}$, there is no such i.

4-34. *[5]* Suppose that you are given a sorted sequence of *distinct* integers $\{a_1, a_2, \ldots, a_n\}$, drawn from 1 to m where $n < m$. Give an $O(\lg n)$ algorithm to find an integer $\leq m$ that is not present in a. For full credit, find the smallest such integer.

4-35. *[5]* Let M be an $n \times m$ integer matrix in which the entries of each row are sorted in increasing order (from left to right) and the entries in each column are in increasing order (from top to bottom). Give an efficient algorithm to find the position of an integer x in M, or to determine that x is not there. How many comparisons of x with matrix entries does your algorithm use in worst case?

Implementation Challenges

4-36. *[5]* Consider an $n \times n$ array A containing integer elements (positive, negative, and zero). Assume that the elements in each row of A are in strictly increasing order, and the elements of each column of A are in strictly decreasing order. (Hence there cannot be two zeroes in the same row or the same column.) Describe an efficient algorithm that counts the number of occurrences of the element 0 in A. Analyze its running time.

4-37. *[6]* Implement versions of several different sorting algorithms, such as selection sort, insertion sort, heapsort, mergesort, and quicksort. Conduct experiments to assess the relative performance of these algorithms in a simple application that reads a large text file and reports exactly one instance of each word that appears within it. This application can be efficiently implemented by sorting all the words that occur in the text and then passing through the sorted sequence to identify one instance of each distinct word. Write a brief report with your conclusions.

4-38. *[5]* Implement an external sort, which uses intermediate files to sort files bigger than main memory. Mergesort is a good algorithm to base such an implementation on. Test your program both on files with small records and on files with large records.

4-39. *[8]* Design and implement a parallel sorting algorithm that distributes data across several processors. An appropriate variation of mergesort is a likely candidate. Measure the speedup of this algorithm as the number of processors increases. Later, compare the execution time to that of a purely sequential mergesort implementation. What are your experiences?

Interview Problems

4-40. *[3]* If you are given a million integers to sort, what algorithm would you use to sort them? How much time and memory would that consume?

4-41. *[3]* Describe advantages and disadvantages of the most popular sorting algorithms.

4-42. *[3]* Implement an algorithm that takes an input array and returns only the unique elements in it.

4-43. *[5]* You have a computer with only 2Mb of main memory. How do you use it to sort a large file of 500 Mb that is on disk?

4-44. *[5]* Design a stack that supports push, pop, and retrieving the minimum element in constant time. Can you do this?

4-45. *[5]* Given a search string of three words, find the smallest snippet of the document that contains all three of the search words—i.e. , the snippet with smallest number of words in it. You are given the index positions where these words in occur search strings, such as *word1: (1, 4, 5)*, *word2: (4, 9, 10)*, and *word3: (5, 6, 15)*. Each of the lists are in sorted order, as above.

4-46. *[6]* You are given 12 coins. One of them is heavier or lighter than the rest. Identify this coin in just three weighings.

Programming Challenges

These programming challenge problems with robot judging are available at *http://www.programming-challenges.com* or *http://online-judge.uva.es*.

4-1. "Vito's Family" – Programming Challenges 110401, UVA Judge 10041.

4-2. "Stacks of Flapjacks" – Programming Challenges 110402, UVA Judge 120.

4-3. "Bridge" – Programming Challenges 110403, UVA Judge 10037.

4-4. "ShoeMaker's Problem" – Programming Challenges 110405, UVA Judge 10026.

4-5. "ShellSort" – Programming Challenges 110407, UVA Judge 10152.

5

Graph Traversal

Graphs are one of the unifying themes of computer science—an abstract representation that describes the organization of transportation systems, human interactions, and telecommunication networks. That so many different structures can be modeled using a single formalism is a source of great power to the educated programmer.

More precisely, a graph $G = (V, E)$ consists of a set of *vertices* V together with a set E of vertex pairs or *edges*. Graphs are important because they can be used to represent essentially *any* relationship. For example, graphs can model a network of roads, with cities as vertices and roads between cities as edges, as shown in Figure 5.1. Electronic circuits can also be modeled as graphs, with junctions as vertices and components as edges.

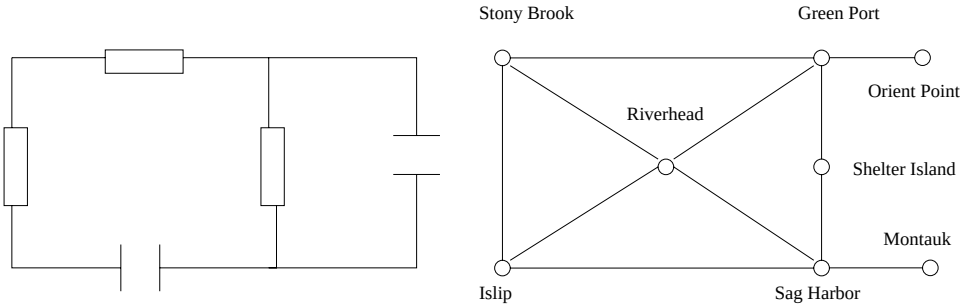

Figure 5.1: Modeling road networks and electronic circuits as graphs

S.S. Skiena, *The Algorithm Design Manual*, 2nd ed., DOI: 10.1007/978-1-84800-070-4_5,
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The key to solving many algorithmic problems is to think of them in terms of graphs. Graph theory provides a language for talking about the properties of relationships, and it is amazing how often messy applied problems have a simple description and solution in terms of classical graph properties.

Designing truly novel graph algorithms is a very difficult task. The key to using graph algorithms effectively in applications lies in correctly modeling your problem so you can take advantage of existing algorithms. Becoming familiar with many different algorithmic graph *problems* is more important than understanding the details of particular graph algorithms, particularly since Part II of this book will point you to an implementation as soon as you know the name of your problem.

Here we present basic data structures and traversal operations for graphs, which will enable you to cobble together solutions for basic graph problems. Chapter 6 will present more advanced graph algorithms that find minimum spanning trees, shortest paths, and network flows, but we stress the primary importance of correctly modeling your problem. Time spent browsing through the catalog now will leave you better informed of your options when a real job arises.

5.1 Flavors of Graphs

A graph $G = (V, E)$ is defined on a set of *vertices* V, and contains a set of *edges* E of ordered or unordered pairs of vertices from V. In modeling a road network, the vertices may represent the cities or junctions, certain pairs of which are connected by roads/edges. In analyzing the source code of a computer program, the vertices may represent lines of code, with an edge connecting lines x and y if y is the next statement executed after x. In analyzing human interactions, the vertices typically represent people, with edges connecting pairs of related souls.

Several fundamental properties of graphs impact the choice of the data structures used to represent them and algorithms available to analyze them. The first step in any graph problem is determining the flavors of graphs you are dealing with:

- *Undirected vs. Directed* – A graph $G = (V, E)$ is *undirected* if edge $(x, y) \in E$ implies that (y, x) is also in E. If not, we say that the graph is *directed*. Road networks *between* cities are typically undirected, since any large road has lanes going in both directions. Street networks *within* cities are almost always directed, because there are at least a few one-way streets lurking somewhere. Program-flow graphs are typically directed, because the execution flows from one line into the next and changes direction only at branches. Most graphs of graph-theoretic interest are undirected.

- *Weighted vs. Unweighted* – Each edge (or vertex) in a *weighted* graph G is assigned a numerical value, or weight. The edges of a road network graph might be weighted with their length, drive-time, or speed limit, depending upon the

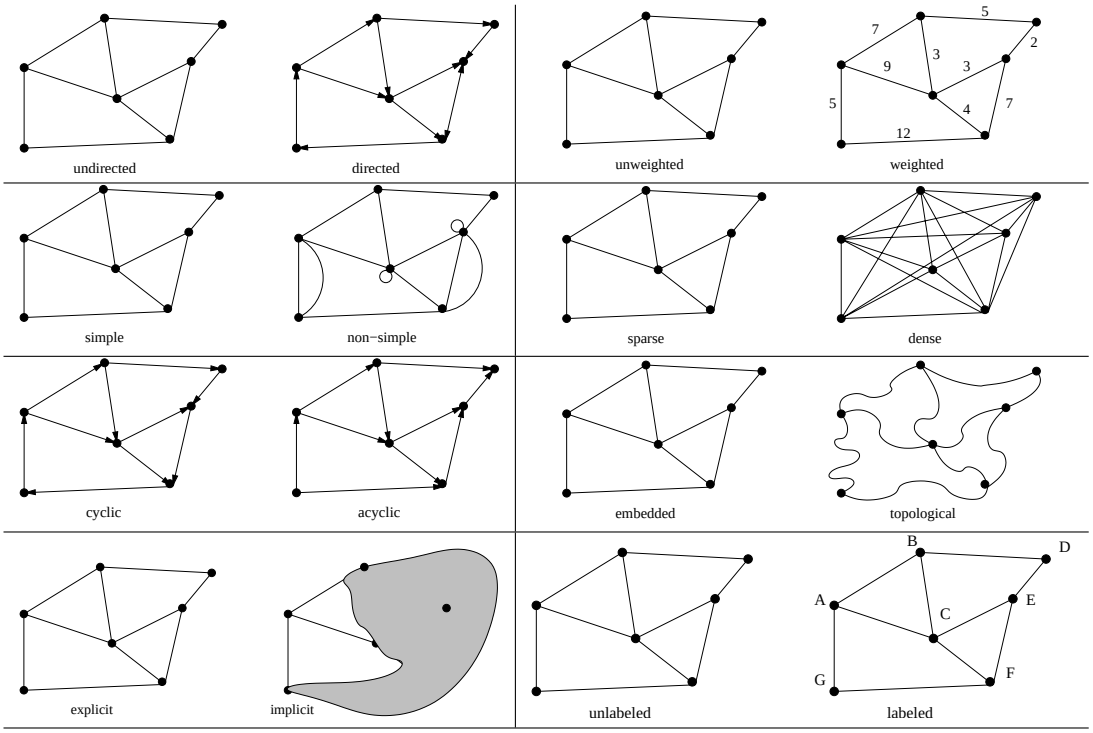


Figure 5.2: Important properties / flavors of graphs

application. In *unweighted* graphs, there is no cost distinction between various edges and vertices.

The difference between weighted and unweighted graphs becomes particularly apparent in finding the shortest path between two vertices. For unweighted graphs, the shortest path must have the fewest number of edges, and can be found using a breadth-first search as discussed in this chapter. Shortest paths in weighted graphs requires more sophisticated algorithms, as discussed in Chapter 6.

- *Simple vs. Non-simple* – Certain types of edges complicate the task of working with graphs. A *self-loop* is an edge (x, x) involving only one vertex. An edge (x, y) is a *multiedge* if it occurs more than once in the graph.

  Both of these structures require special care in implementing graph algorithms. Hence any graph that avoids them is called *simple*.

- *Sparse vs. Dense*: Graphs are *sparse* when only a small fraction of the possible vertex pairs ($\binom{n}{2}$ for a simple, undirected graph on n vertices) actually have edges defined between them. Graphs where a large fraction of the vertex pairs define edges are called *dense*. There is no official boundary between what is called sparse and what is called dense, but typically dense graphs have a quadratic number of edges, while sparse graphs are linear in size.

  Sparse graphs are usually sparse for application-specific reasons. Road networks must be sparse graphs because of road junctions. The most ghastly intersection I've ever heard of was the endpoint of only seven different roads. Junctions of electrical components are similarly limited to the number of wires that can meet at a point, perhaps except for power and ground.

- *Cyclic vs. Acyclic* – An *acyclic* graph does not contain any cycles. *Trees* are connected, acyclic undirected graphs. Trees are the simplest interesting graphs, and are inherently recursive structures because cutting any edge leaves two smaller trees.

  Directed acyclic graphs are called *DAGs*. They arise naturally in scheduling problems, where a directed edge (x, y) indicates that activity x must occur before y. An operation called *topological sorting* orders the vertices of a DAG to respect these precedence constraints. Topological sorting is typically the first step of any algorithm on a DAG, as will be discussed in Section 5.10.1 (page 179).

- *Embedded vs. Topological* – A graph is *embedded* if the vertices and edges are assigned geometric positions. Thus, any drawing of a graph is an *embedding*, which may or may not have algorithmic significance.

  Occasionally, the structure of a graph is completely defined by the geometry of its embedding. For example, if we are given a collection of points in the plane, and seek the minimum cost tour visiting all of them (i.e., the traveling salesman problem), the underlying topology is the *complete graph* connecting each pair of vertices. The weights are typically defined by the Euclidean distance between each pair of points.

  Grids of points are another example of topology from geometry. Many problems on an $n \times m$ grid involve walking between neighboring points, so the edges are implicitly defined from the geometry.

- *Implicit vs. Explicit* – Certain graphs are not explicitly constructed and then traversed, but built as we use them. A good example is in backtrack search. The vertices of this implicit search graph are the states of the search vector, while edges link pairs of states that can be directly generated from each other. Because you do not have to store the entire graph, it is often easier to work with an implicit graph than explicitly construct it prior to analysis.

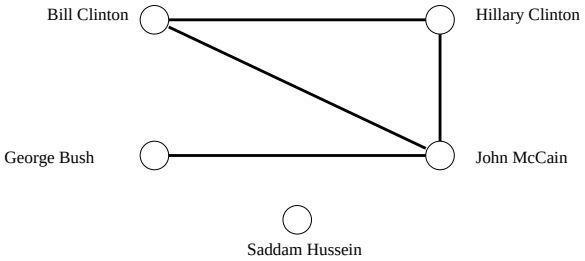


Figure 5.3: A portion of the friendship graph

- *Labeled vs. Unlabeled* – Each vertex is assigned a unique name or identifier in a *labeled* graph to distinguish it from all other vertices. In *unlabeled* graphs, no such distinctions have been made.

  Graphs arising in applications are often naturally and meaningfully labeled, such as city names in a transportation network. A common problem is that of *isomorphism testing*—determining whether the topological structure of two graphs are identical if we ignore any labels. Such problems are typically solved using backtracking, by trying to assign each vertex in each graph a label such that the structures are identical.

5.1.1 The Friendship Graph

To demonstrate the importance of proper modeling, let us consider a graph where the vertices are people, and there is an edge between two people if and only if they are friends. Such graphs are called *social networks* and are well defined on any set of people—be they the people in your neighborhood, at your school/business, or even spanning the entire world. An entire science analyzing social networks has sprung up in recent years, because many interesting aspects of people and their behavior are best understood as properties of this friendship graph.

Most of the graphs that one encounters in real life are sparse. The friendship graph is good example. Even the most gregarious person on earth knows an insignificant fraction of the world's population.

We use this opportunity to demonstrate the graph theory terminology described above. "Talking the talk" proves to be an important part of "walking the walk":

- *If I am your friend, does that mean you are my friend?* – This question really asks whether the graph is directed. A graph is *undirected* if edge (x, y) always implies (y, x). Otherwise, the graph is said to be *directed*. The "heard-of" graph is directed, since I have heard of many famous people who have never heard of me! The "had-sex-with" graph is presumably undirected, since the critical operation always requires a partner. I'd like to think that the "friendship" graph is also an undirected graph.

- *How close a friend are you?* – In *weighted* graphs, each edge has an associated numerical attribute. We could model the strength of a friendship by associating each edge with an appropriate value, perhaps from -10 (enemies) to 10 (blood brothers). The edges of a road network graph might be weighted with their length, drive-time, or speed limit, depending upon the application. A graph is said to be *unweighted* if all edges are assumed to be of equal weight.

- *Am I my own friend?* – This question addresses whether the graph is *simple*, meaning it contains no loops and no multiple edges. An edge of the form (x, x) is said to be a *loop*. Sometimes people are friends in several different ways. Perhaps x and y were college classmates and now work together at the same company. We can model such relationships using *multiedges*—multiple edges (x, y) perhaps distinguished by different labels.

  Simple graphs really are often simpler to work with in practice. Therefore, we might be better off declaring that no one is their own friend.

- *Who has the most friends?* – The *degree* of a vertex is the number of edges adjacent to it. The most popular person defines the vertex of highest degree in the friendship graph. Remote hermits are associated with degree-zero vertices.

  In *dense* graphs, most vertices have high degrees, as opposed to *sparse* graphs with relatively few edges. In a *regular graph*, each vertex has exactly the same degree. A regular friendship graph is truly the ultimate in social-ism.

- *Do my friends live near me?* – Social networks are not divorced from geography. Many of your friends are your friends only because they happen to live near you (e.g., neighbors) or used to live near you (e.g., college roommates).

  Thus, a full understanding of social networks requires an *embedded* graph, where each vertex is associated with the point on this world where they live. This geographic information may not be explicitly encoded, but the fact that the graph is inherently embedded in the plane shapes our interpretation of any analysis.

- *Oh, you also know her?* – Social networking services such as Myspace and LinkedIn are built on the premise of *explicitly* defining the links between members and their member-friends. Such graphs consist of directed edges from person/vertex x professing his friendship to person/vertex y.

  That said, the complete friendship graph of the world is represented *implicitly*. Each person knows who their friends are, but cannot find out about other people's friendships except by asking them. The "six degrees of separation" theory argues that there is a short path linking every two people in the world (e.g., Skiena and the President) but offers us no help in actually finding this path. The shortest such path I know of contains three hops (Steven Skiena → Bob McGrath → John Marberger → George W. Bush), but there could

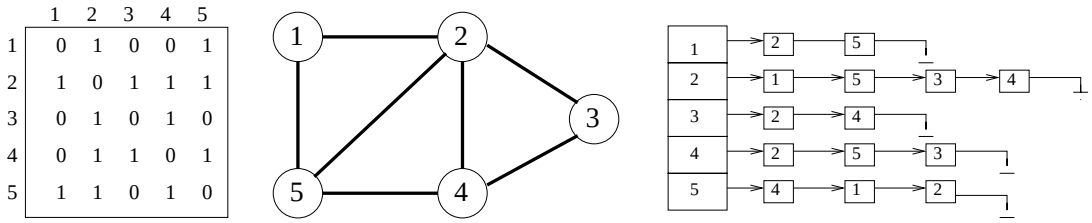


Figure 5.4: The adjacency matrix and adjacency list of a given graph

be a shorter one (say, if he went to college with my dentist). The friendship graph is stored implicitly, so I have no way of easily checking.

- *Are you truly an individual, or just one of the faceless crowd?* – This question boils down to whether the friendship graph is labeled or unlabeled. Does each vertex have a name/label which reflects its identify, and is this label important for our analysis?

  Much of the study of social networks is unconcerned with labels on graphs. Often the index number given a vertex in the graph data structure serves as its label, perhaps for convenience or the need for anonymity. You may assert that you are a name, not a number—but try protesting to the guy who implements the algorithm. Someone studying how an infectious disease spreads through a graph may label each vertex with whether the person is healthy or sick, it being irrelevant what their name is.

Take-Home Lesson: Graphs can be used to model a wide variety of structures and relationships. Graph-theoretic terminology gives us a language to talk about them.

5.2 Data Structures for Graphs

Selecting the right graph data structure can have an enormous impact on performance. Your two basic choices are adjacency matrices and adjacency lists, illustrated in Figure 5.4. We assume the graph $G = (V, E)$ contains n vertices and m edges.

- *Adjacency Matrix*: We can represent G using an $n \times n$ matrix M, where element $M[i, j] = 1$ if (i, j) is an edge of G, and 0 if it isn't. This allows fast answers to the question "is (i, j) in G?", and rapid updates for edge insertion and deletion. It may use excessive space for graphs with many vertices and relatively few edges, however.

Comparison	Winner
Faster to test if (x, y) is in graph?	adjacency matrices
Faster to find the degree of a vertex?	adjacency lists
Less memory on small graphs?	adjacency lists $(m + n)$ vs. (n^2)
Less memory on big graphs?	adjacency matrices (a small win)
Edge insertion or deletion?	adjacency matrices $O(1)$ vs. $O(d)$
Faster to traverse the graph?	adjacency lists $\Theta(m + n)$ vs. $\Theta(n^2)$
Better for most problems?	adjacency lists

Figure 5.5: Relative advantages of adjacency lists and matrices.

Consider a graph that represents the street map of Manhattan in New York City. Every junction of two streets will be a vertex of the graph. Neighboring junctions are connected by edges. How big is this graph? Manhattan is basically a grid of 15 avenues each crossing roughly 200 streets. This gives us about 3,000 vertices and 6,000 edges, since each vertex neighbors four other vertices and each edge is shared between two vertices. This modest amount of data should easily and efficiently be stored, yet an adjacency matrix would have $3{,}000 \times 3{,}000 = 9{,}000{,}000$ cells, almost all of them empty!

There is some potential to save space by packing multiple bits per word or simulating a triangular matrix on undirected graphs. But these methods lose the simplicity that makes adjacency matrices so appealing and, more critically, remain inherently quadratic on sparse graphs.

- *Adjacency Lists*: We can more efficiently represent sparse graphs by using linked lists to store the neighbors adjacent to each vertex. Adjacency lists require pointers but are not frightening once you have experience with linked structures.

  Adjacency lists make it harder to verify whether a given edge (i, j) is in G, since we must search through the appropriate list to find the edge. However, it is surprisingly easy to design graph algorithms that avoid any need for such queries. Typically, we sweep through all the edges of the graph in one pass via a breadth-first or depth-first traversal, and update the implications of the current edge as we visit it. Table 5.5 summarizes the tradeoffs between adjacency lists and matrices.

Take-Home Lesson: Adjacency lists are the right data structure for most applications of graphs.

We will use adjacency lists as our primary data structure to represent graphs. We represent a graph using the following data type. For each graph, we keep a

count of the number of vertices, and assign each vertex a unique identification number from 1 to `nvertices`. We represent the edges using an array of linked lists:

```
#define MAXV            1000        /* maximum number of vertices */

typedef struct {
        int y;                      /* adjacency info */
        int weight;                 /* edge weight, if any */
        struct edgenode *next;      /* next edge in list */
} edgenode;


typedef struct {
        edgenode *edges[MAXV+1];    /* adjacency info */
        int degree[MAXV+1];         /* outdegree of each vertex */
        int nvertices;              /* number of vertices in graph */
        int nedges;                 /* number of edges in graph */
        bool directed;              /* is the graph directed? */
} graph;
```

We represent directed edge (x, y) by an `edgenode` y in x's adjacency list. The degree field of the `graph` counts the number of meaningful entries for the given vertex. An undirected edge (x, y) appears twice in any adjacency-based graph structure, once as y in x's list, and once as x in y's list. The boolean flag `directed` identifies whether the given graph is to be interpreted as directed or undirected.

To demonstrate the use of this data structure, we show how to read a graph from a file. A typical graph format consists of an initial line featuring the number of vertices and edges in the graph, followed by a listing of the edges at one vertex pair per line.

```
initialize_graph(graph *g, bool directed)
{
        int i;                          /* counter */

        g -> nvertices = 0;
        g -> nedges = 0;
        g -> directed = directed;

        for (i=1; i<=MAXV; i++) g->degree[i] = 0;
        for (i=1; i<=MAXV; i++) g->edges[i] = NULL;
}
```

Actually reading the graph requires inserting each edge into this structure:

```
read_graph(graph *g, bool directed)
{
        int i;                          /* counter */
        int m;                          /* number of edges */
        int x, y;                       /* vertices in edge (x,y) */

        initialize_graph(g, directed);

        scanf("%d %d",&(g->nvertices),&m);

        for (i=1; i<=m; i++) {
                scanf("%d %d",&x,&y);
                insert_edge(g,x,y,directed);
        }
}
```

The critical routine is `insert_edge`. The new `edgenode` is inserted at the beginning of the appropriate adjacency list, since order doesn't matter. We parameterize our insertion with the `directed` Boolean flag, to identify whether we need to insert two copies of each edge or only one. Note the use of recursion to solve this problem:

```
insert_edge(graph *g, int x, int y, bool directed)
{
      edgenode *p;                  /* temporary pointer */

      p = malloc(sizeof(edgenode)); /* allocate edgenode storage */

      p->weight = NULL;
      p->y = y;
      p->next = g->edges[x];

      g->edges[x] = p;              /* insert at head of list */

      g->degree[x] ++;

      if (directed == FALSE)
              insert_edge(g,y,x,TRUE);
      else
              g->nedges ++;
}
```

Printing the associated graph is just a matter of two nested loops, one through vertices, the other through adjacent edges:

```
print_graph(graph *g)
{
        int i;                          /* counter */
        edgenode *p;                    /* temporary pointer */

        for (i=1; i<=g->nvertices; i++) {
                printf("%d: ",i);
                p = g->edges[i];
                while (p != NULL) {
                        printf(" %d",p->y);
                        p = p->next;
                }
                printf("\n");
        }
}
```

It is a good idea to use a well-designed graph data type as a model for building your own, or even better as the foundation for your application. We recommend LEDA (see Section 19.1.1 (page 658)) or Boost (see Section 19.1.3 (page 659)) as the best-designed general-purpose graph data structures currently available. They may be more powerful (and hence somewhat slower/larger) than you need, but they do so many things right that you are likely to lose most of the potential do-it-yourself benefits through clumsiness.

5.3 War Story: I was a Victim of Moore's Law

I am the author of a popular library of graph algorithms called *Combinatorica* (see *www.combinatorica.com*), which runs under the computer algebra system *Mathematica*. Efficiency is a great challenge in *Mathematica*, due to its applicative model of computation (it does not support constant-time write operations to arrays) and the overhead of interpretation (as opposed to compilation). *Mathematica* code is typically 1,000 to 5,000 times slower than C code.

Such slow downs can be a tremendous performance hit. Even worse, *Mathematica* was a memory hog, needing a then-outrageous 4MB of main memory to run effectively when I completed *Combinatorica* in 1990. Any computation on large structures was doomed to thrash in virtual memory. In such an environment, my graph package could only hope to work effectively on *very* small graphs.

One design decision I made as a result was to use adjacency matrices as the basic *Combinatorica* graph data structure instead of lists. This may sound peculiar. If pressed for memory, wouldn't it pay to use adjacency lists and conserve every last byte? Yes, but the answer is not so simple for very small graphs. An adjacency list representation of a weighted n-vertex, m-edge graph should use about $n+2m$ words to represent; the $2m$ comes from storing the endpoint and weight components of

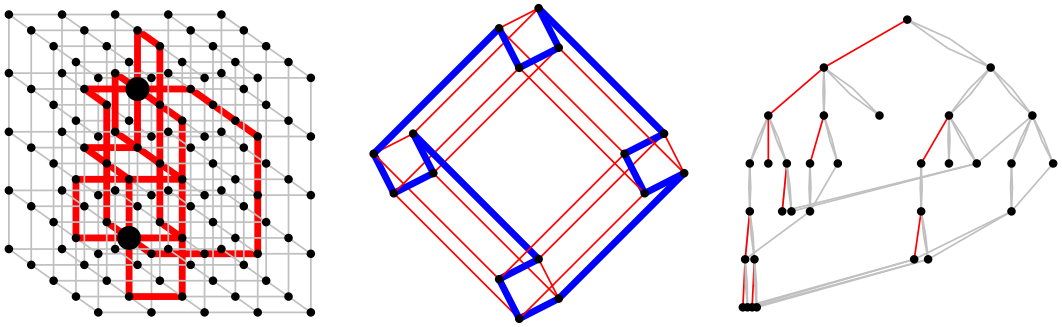


Figure 5.6: Representative *Combinatorica* graphs: edge-disjoint paths (left), Hamiltonian cycle in a hypercube (center), animated depth-first search tree traversal (right)

each edge. Thus, the space advantages of adjacency lists kick in when $n + 2m$ is substantially smaller than n^2. The adjacency matrix is still manageable in size for $n \leq 100$ and, of course, half the size of adjacency lists on dense graphs.

My more immediate concern was dealing with the overhead of using a slow interpreted language. Check out the benchmarks reported in Table 5.1. Two particularly complex but polynomial-time problems on 9 and 16 vertex graphs took several minutes to complete on my desktop machine in 1990! The quadratic-sized data structure certainly could not have had much impact on these running times, since 9×9 equals only 81. From experience, I knew the *Mathematica* programming language handled better to regular structures like adjacency matrices better than irregular-sized adjacency lists.

Still, *Combinatorica* proved to be a very good thing despite these performance problems. Thousands of people have used my package to do all kinds of interesting things with graphs. *Combinatorica* was never intended to be a high-performance algorithms library. Most users quickly realized that computations on large graphs were out of the question, but were eager to take advantage of *Combinatorica* as a mathematical research tool and prototyping environment. Everyone was happy.

But over the years, my users started asking why it took so long to do a modest-sized graph computation. The mystery wasn't that my program was slow, because it had always been slow. The question was why did it take so many years for people to figure this out?

Approximate year command/machine	1990 Sun-3	1991 Sun-4	1998 Sun-5	2000 Ultra 5	2004 SunBlade
PlanarQ[GridGraph[4,4]]	234.10	69.65	27.50	3.60	0.40
Length[Partitions[30]]	289.85	73.20	24.40	3.44	1.58
VertexConnectivity[GridGraph[3,3]]	239.67	47.76	14.70	2.00	0.91
RandomPartition[1000]	831.68	267.5	22.05	3.12	0.87

Table 5.1: Old *Combinatorica* benchmarks on low-end Sun workstations, from 1990 to today, (running time in seconds)

The reason is that computers keep doubling in speed every two years or so. People's *expectation* of how long something should take moves in concert with these technology improvements. Partially because of *Combinatorica*'s dependence on a quadratic-size graph data structure, it didn't scale as well as it should on sparse graphs.

As the years rolled on, user demands become more insistent. *Combinatorica* needed to be updated. My collaborator, Sriram Pemmaraju, rose to the challenge. We (mostly he) completely rewrote *Combinatorica* to take advantage of faster graph data structures ten years after the initial version.

The new *Combinatorica* uses a list of edges data structure for graphs, largely motivated by increased efficiency. Edge lists are linear in the size of the graph (edges plus vertices), just like adjacency lists. This makes a huge difference on most graph related functions—for large enough graphs. The improvement is most dramatic in "fast" graph algorithms—those that run in linear or near linear-time, such as graph traversal, topological sort, and finding connected/biconnected components. The implications of this change is felt throughout the package in running time improvements and memory savings. *Combinatorica* can now work with graphs that are about 50-100 times larger than graphs that the old package could deal with.

Figure 5.7(l) plots the running time of the `MinimumSpanningTree` functions for both *Combinatorica* versions. The test graphs were sparse (grid graphs), designed to highlight the difference between the two data structures. Yes, the new version is *much* faster, but note that the difference only becomes important for graphs larger than the old *Combinatorica* was designed for. However, the relative difference in run time keeps growing with increasing n. Figure 5.7(r) plots the ratio of the running times as a function of graph size. The difference between linear size and quadratic size is asymptotic, so the consequences become ever more important as n gets larger.

What is the weird bump in running times that occurs around $n \approx 250$? This likely reflects a transition between levels of the memory hierarchy. Such bumps are not uncommon in today's complex computer systems. Cache performance in data structure design should be an important but not overriding consideration.

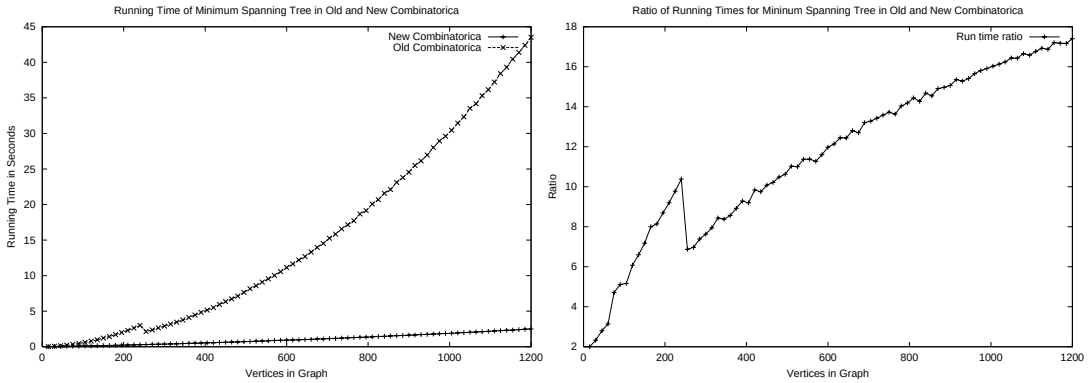


Figure 5.7: Performance comparison between old and new Combinatorica: absolute running times (l), and the ratio of these times (r).

The asymptotic gains due to adjacency lists more than trumped any impact of the cache.

Two main lessons can be taken away from our experience developing *Combinatorica*:

- *To make a program run faster, just wait* – Sophisticated hardware eventually slithers down to everybody. We observe a speedup of more than 200-fold for the original version of *Combinatorica* as a consequence of 15 years of faster hardware. In this context, the further speedups we obtained from upgrading the package become particularly dramatic.

- *Asymptotics eventually do matter* – It was my mistake not to anticipate future developments in technology. While no one has a crystal ball, it is fairly safe to say that future computers will have more memory and run faster than today's. This gives an edge to asymptotically more efficient algorithms/data structures, even if their performance is close on today's instances. If the implementation complexity is not substantially greater, play it safe and go with the better algorithm.

5.4 War Story: Getting the Graph

"It takes five minutes just to *read* the data. We will *never* have time to make it do something interesting."

The young graduate student was bright and eager, but green to the power of data structures. She would soon come to appreciate their power.

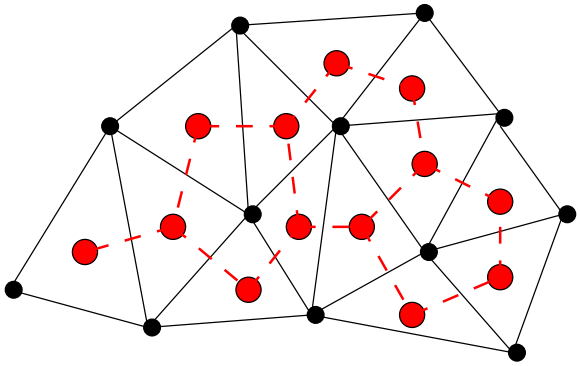


Figure 5.8: The dual graph (dashed lines) of a triangulation

As described in a previous war story (see Section 3.6 (page 85)), we were experimenting with algorithms to extract triangular strips for the fast rendering of triangulated surfaces. The task of finding a small number of strips that cover each triangle in a mesh could be modeled as a graph problem. The graph has a vertex for every *triangle* of the mesh, with an edge between every pair of vertices representing adjacent triangles. This *dual graph* representation (see Figure 5.8) captures all the information needed to partition the triangulation into triangle strips.

The first step in crafting a program that constructs a good set of strips was to build the dual graph of the triangulation. This I sent the student off to do. A few days later, she came back and announced that it took over five CPU minutes just to construct this dual graph of a few thousand triangles.

"Nonsense!" I proclaimed. "You must be doing something very wasteful in building the graph. What format is the data in?"

"Well, it starts out with a list of the 3D coordinates of the vertices used in the model and then follows with a list of triangles. Each triangle is described by a list of three indices into the vertex coordinates. Here is a small example:"

```
VERTICES 4
0.000000 240.000000 0.000000
204.000000 240.000000 0.000000
204.000000 0.000000 0.000000
0.000000 0.000000 0.000000
TRIANGLES 2
0 1 3
1 2 3
```

"I see. So the first triangle uses all but the third point, since all the indices start from zero. The two triangles must share an edge formed by points 1 and 3."

"Yeah, that's right," she confirmed.

"OK. Now tell me how you built your dual graph from this file."

"Well, I can ignore the vertex information once I know how many vertices there are. The geometric position of the points doesn't affect the structure of the graph. My dual graph is going to have as many vertices as the number of triangles. I set up an adjacency list data structure with that many vertices. As I read in each triangle, I compare it to each of the others to check whether it has two end points in common. If it does, I add an edge from the new triangle to this one."

I started to sputter. "But *that's* your problem right there! You are comparing each triangle against every other triangle, so that constructing the dual graph will be quadratic in the number of triangles. Reading the input graph should take linear time!"

"I'm not comparing every triangle against every other triangle. On average, it only tests against half or a third of the triangles."

"Swell. But that still leaves us with an $O(n^2)$ algorithm. That is much too slow."

She stood her ground. "Well, don't just complain. Help me fix it!"

Fair enough. I started to think. We needed some quick method to screen away most of the triangles that would not be adjacent to the new triangle (i, j, k). What we really needed was a separate list of all the triangles that go through each of the points i, j, and k. By Euler's formula for planar graphs, the average point is incident on less than six triangles. This would compare each new triangle against fewer than twenty others, instead of most of them.

"We are going to need a data structure consisting of an array with one element for every vertex in the original data set. This element is going to be a list of all the triangles that pass through that vertex. When we read in a new triangle, we will look up the three relevant lists in the array and compare each of these against the new triangle. Actually, only two of the three lists need be tested, since any adjacent triangles will share two points in common. We will add an adjacency to our graph for every triangle-pair sharing two vertices. Finally, we will add our new triangle to each of the three affected lists, so they will be updated for the next triangle read."

She thought about this for a while and smiled. "Got it, Chief. I'll let you know what happens."

The next day she reported that the graph could be built in seconds, even for much larger models. From here, she went on to build a successful program for extracting triangle strips, as reported in Section 3.6 (page 85).

The take-home lesson is that even elementary problems like initializing data structures can prove to be bottlenecks in algorithm development. Most programs working with large amounts of data have to run in linear or almost linear time. Such tight performance demands leave no room to be sloppy. Once you focus on the need for linear-time performance, an appropriate algorithm or heuristic can usually be found to do the job.

5.5 Traversing a Graph

Perhaps the most fundamental graph problem is to visit every edge and vertex in a graph in a systematic way. Indeed, all the basic bookkeeping operations on graphs (such printing or copying graphs, and converting between alternate representations) are applications of graph traversal.

Mazes are naturally represented by graphs, where each graph vertex denotes a junction of the maze, and each graph edge denotes a hallway in the maze. Thus, any graph traversal algorithm must be powerful enough to get us out of an arbitrary maze. For *efficiency*, we must make sure we don't get trapped in the maze and visit the same place repeatedly. For *correctness*, we must do the traversal in a systematic way to guarantee that we get out of the maze. Our search must take us through every edge and vertex in the graph.

The key idea behind graph traversal is to mark each vertex when we first visit it and keep track of what we have not yet completely explored. Although bread crumbs or unraveled threads have been used to mark visited places in fairy-tale mazes, we will rely on Boolean flags or enumerated types.

Each vertex will exist in one of three states:

- *undiscovered* – the vertex is in its initial, virgin state.
- *discovered* – the vertex has been found, but we have not yet checked out all its incident edges.
- *processed* – the vertex after we have visited all its incident edges.

Obviously, a vertex cannot be *processed* until after we discover it, so the state of each vertex progresses over the course of the traversal from *undiscovered* to *discovered* to *processed*.

We must also maintain a structure containing the vertices that we have discovered but not yet completely processed. Initially, only the single start vertex is considered to be discovered. To completely explore a vertex v, we must evaluate each edge leaving v. If an edge goes to an undiscovered vertex x, we mark x *discovered* and add it to the list of work to do. We ignore an edge that goes to a *processed* vertex, because further contemplation will tell us nothing new about the graph. We can also ignore any edge going to a *discovered* but not *processed* vertex, because the destination already resides on the list of vertices to process.

Each undirected edge will be considered exactly twice, once when each of its endpoints is explored. Directed edges will be considered only once, when exploring the source vertex. Every edge and vertex in the connected component must eventually be visited. Why? Suppose that there exists a vertex u that remains unvisited, whose neighbor v *was* visited. This neighbor v will eventually be explored, after which we will certainly visit u. Thus, we must find everything that is there to be found.

We describe the mechanics of these traversal algorithms and the significance of the traversal order below.

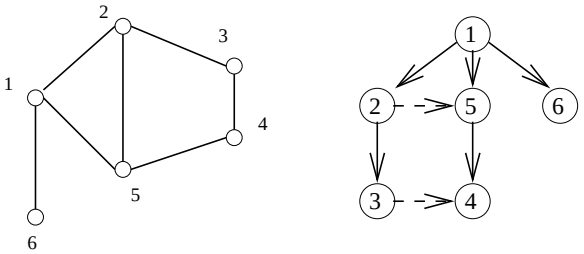


Figure 5.9: An undirected graph and its breadth-first search tree

5.6 Breadth-First Search

The basic breadth-first search algorithm is given below. At some point during the course of a traversal, every node in the graph changes state from *undiscovered* to *discovered*. In a breadth-first search of an undirected graph, we assign a direction to each edge, from the discoverer u to the discovered v. We thus denote u to be the parent of v. Since each node has exactly one parent, except for the root, this defines a tree on the vertices of the graph. This tree, illustrated in Figure 5.9, defines a shortest path from the root to every other node in the tree. This property makes breadth-first search very useful in shortest path problems.

```
BFS(G, s)
    for each vertex u ∈ V[G] − {s} do
        state[u] = "undiscovered"
        p[u] = nil, i.e. no parent is in the BFS tree
    state[s] = "discovered"
    p[s] = nil
    Q = {s}
    while Q ≠ ∅ do
        u = dequeue[Q]
        process vertex u as desired
        for each v ∈ Adj[u] do
            process edge (u, v) as desired
            if state[v] = "undiscovered" then
                state[v] = "discovered"
                p[v] = u
                enqueue[Q, v]
        state[u] = "processed"
```

The graph edges that do not appear in the breadth-first search tree also have special properties. For undirected graphs, nontree edges can point only to vertices on the same level as the parent vertex, or to vertices on the level directly below

the parent. These properties follow easily from the fact that each path in the tree must be the shortest path in the graph. For a directed graph, a back-pointing edge (u, v) can exist whenever v lies closer to the root than u does.

Implementation

Our breadth-first search implementation `bfs` uses two Boolean arrays to maintain our knowledge about each vertex in the graph. A vertex is `discovered` the first time we visit it. A vertex is considered `processed` after we have traversed all outgoing edges from it. Thus, each vertex passes from undiscovered to discovered to processed over the course of the search. This information could have been maintained using one enumerated type variable, but we used two Boolean variables instead.

```
bool processed[MAXV+1];   /* which vertices have been processed */
bool discovered[MAXV+1];  /* which vertices have been found */
int parent[MAXV+1];       /* discovery relation */
```

Each vertex is initialized as undiscovered:

```
initialize_search(graph *g)
{
        int i;                          /* counter */

        for (i=1; i<=g->nvertices; i++) {
                processed[i] = discovered[i] = FALSE;
                parent[i] = -1;
        }
}
```

Once a vertex is discovered, it is placed on a queue. Since we process these vertices in first-in, first-out order, the oldest vertices are expanded first, which are exactly those closest to the root:

```
bfs(graph *g, int start)
{
        queue q;                    /* queue of vertices to visit */
        int v;                      /* current vertex */
        int y;                      /* successor vertex */
        edgenode *p;                /* temporary pointer */

        init_queue(&q);
        enqueue(&q,start);
        discovered[start] = TRUE;
```

```
        while (empty_queue(&q) == FALSE) {
                v = dequeue(&q);
                process_vertex_early(v);
                processed[v] = TRUE;
                p = g->edges[v];
                while (p != NULL) {
                    y = p->y;
                    if ((processed[y] == FALSE) || g->directed)
                        process_edge(v,y);
                    if (discovered[y] == FALSE) {
                        enqueue(&q,y);
                        discovered[y] = TRUE;
                        parent[y] = v;
                    }
                    p = p->next;
                }
                process_vertex_late(v);
        }
}
```

5.6.1 Exploiting Traversal

The exact behavior of `bfs` depends upon the functions `process_vertex_early()`, `process_vertex_late()`, and `process_edge()`. Through these functions, we can customize what the traversal does as it makes its official visit to each edge and each vertex. Initially, we will do all of vertex processing on entry, so `process_vertex_late()` returns without action:

```
process_vertex_late(int v)
{
}
```

By setting the active functions to

```
process_vertex_early(int v)
{
        printf("processed vertex %d\n",v);
}


process_edge(int x, int y)
{
        printf("processed edge (%d,%d)\n",x,y);
}
```

we print each vertex and edge exactly once. If we instead set `process_edge` to

```
process_edge(int x, int y)
{
        nedges = nedges + 1;
}
```

we get an accurate count of the number of edges. Different algorithms perform different actions on vertices or edges as they are encountered. These functions give us the freedom to easily customize our response.

5.6.2 Finding Paths

The `parent` array set within `bfs()` is very useful for finding interesting paths through a graph. The vertex that discovered vertex i is defined as `parent[i]`. Every vertex is discovered during the course of traversal, so except for the root every node has a parent. The parent relation defines a tree of discovery with the initial search node as the root of the tree.

Because vertices are discovered in order of increasing distance from the root, this tree has a very important property. The unique tree path from the root to each node $x \in V$ uses the smallest number of edges (or equivalently, intermediate nodes) possible on any root-to-x path in the graph.

We can reconstruct this path by following the chain of ancestors from x to the root. Note that we have to work backward. We cannot find the path from the root to x, since that does not follow the direction of the parent pointers. Instead, we must find the path from x to the root. Since this is the reverse of how we normally want the path, we can either (1) store it and then explicitly reverse it using a stack, or (2) let recursion reverse it for us, as follows:

```
find_path(int start, int end, int parents[])
{
        if ((start == end) || (end == -1))
                printf("\n%d",start);
        else {
                find_path(start,parents[end],parents);
                printf(" %d",end);
        }
}
```

On our breadth-first search graph example (Figure 5.9) our algorithm generated the following parent relation:

vertex	1	2	3	4	5	6
parent	-1	1	2	5	1	1

For the shortest path from 1 to 4, upper-right corner, this parent relation yields the path $\{1, 5, 4\}$.

There are two points to remember when using breadth-first search to find a shortest path from x to y: First, the shortest path tree is only useful if BFS was performed with x as the root of the search. Second, BFS gives the shortest path only if the graph is unweighted. We will present algorithms for finding shortest paths in weighted graphs in Section 6.3.1 (page 206).

5.7 Applications of Breadth-First Search

Most elementary graph algorithms make one or two traversals of the graph while we update our knowledge of the graph. Properly implemented using adjacency lists, any such algorithm is destined to be linear, since BFS runs in $O(n + m)$ time on both directed and undirected graphs. This is optimal, since it is as fast as one can hope to *read* any n-vertex, m-edge graph.

The trick is seeing when traversal approaches are destined to work. We present several examples below.

5.7.1 Connected Components

The "six degrees of separation" theory argues that there is always a short path linking every two people in the world. We say that a graph is *connected* if there is a path between any two vertices. If the theory is true, it means the friendship graph must be connected.

A *connected component* of an undirected graph is a maximal set of vertices such that there is a path between every pair of vertices. The components are separate "pieces" of the graph such that there is no connection between the pieces. If we envision tribes in remote parts of the world that have yet not been encountered, each such tribe would form a separate connected component in the friendship graph. A remote hermit, or extremely unpleasant fellow, would represent a connected component of one vertex.

An amazing number of seemingly complicated problems reduce to finding or counting connected components. For example, testing whether a puzzle such as Rubik's cube or the 15-puzzle can be solved from any position is really asking whether the graph of legal configurations is connected.

Connected components can be found using breadth-first search, since the vertex order does not matter. We start from the first vertex. Anything we discover during this search must be part of the same connected component. We then repeat the search from any undiscovered vertex (if one exists) to define the next component, and so on until all vertices have been found:

```
connected_components(graph *g)
{
        int c;                          /* component number */
        int i;                          /* counter */

        initialize_search(g);

        c = 0;
        for (i=1; i<=g->nvertices; i++)
                if (discovered[i] == FALSE) {
                        c = c+1;
                        printf("Component %d:",c);
                        bfs(g,i);
                        printf("\n");
                }
}


process_vertex_early(int v)
{
        printf(" %d",v);
}


process_edge(int x, int y)
{
}
```

Observe how we increment a counter c denoting the current component number with each call to `bfs`. We could have explicitly bound each vertex to its component number (instead of printing the vertices in each component) by changing the action of `process_vertex`.

There are two distinct notions of connectivity for directed graphs, leading to algorithms for finding both weakly connected and strongly connected components. Both of these can be found in $O(n + m)$ time, as discussed in Section 15.1 (page 477).

5.7.2 Two-Coloring Graphs

The *vertex-coloring* problem seeks to assign a label (or color) to each vertex of a graph such that no edge links any two vertices of the same color. We can easily avoid all conflicts by assigning each vertex a unique color. However, the goal is to use as few colors as possible. Vertex coloring problems often arise in scheduling applications, such as register allocation in compilers. See Section 16.7 (page 544) for a full treatment of vertex-coloring algorithms and applications.

A graph is *bipartite* if it can be colored without conflicts while using only two colors. Bipartite graphs are important because they arise naturally in many applications. Consider the "had-sex-with" graph in a heterosexual world. Men have sex only with women, and vice versa. Thus, gender defines a legal two-coloring, in this simple model.

But how can we find an appropriate two-coloring of a graph, thus separating the men from the women? Suppose we assume that the starting vertex is male. All vertices adjacent to this man must be female, assuming the graph is indeed bipartite.

We can augment breadth-first search so that whenever we discover a new vertex, we color it the opposite of its parent. We check whether any nondiscovery edge links two vertices of the same color. Such a conflict means that the graph cannot be two-colored. Otherwise, we will have constructed a proper two-coloring whenever we terminate without conflict.

```
twocolor(graph *g)
{
        int i;                          /* counter */

        for (i=1; i<=(g->nvertices); i++)
                color[i] = UNCOLORED;

        bipartite = TRUE;

        initialize_search(&g);

        for (i=1; i<=(g->nvertices); i++)
                if (discovered[i] == FALSE) {
                        color[i] = WHITE;
                        bfs(g,i);
                }
}


process_edge(int x, int y)
{
     if (color[x] == color[y]) {
             bipartite = FALSE;
             printf("Warning: not bipartite due to (%d,%d)\n",x,y);
     }

     color[y] = complement(color[x]);
}
```

```
complement(int color)
{
        if (color == WHITE) return(BLACK);
        if (color == BLACK) return(WHITE);

        return(UNCOLORED);
}
```

We can assign the first vertex in any connected component to be whatever color/sex we wish. BFS can separate the men from the women, but we can't tell them apart just by using the graph structure.

Take-Home Lesson: Breadth-first and depth-first searches provide mechanisms to visit each edge and vertex of the graph. They prove the basis of most simple, efficient graph algorithms.

5.8 Depth-First Search

There are two primary graph traversal algorithms: *breadth-first search* (BFS) and *depth-first search* (DFS). For certain problems, it makes absolutely no difference which you use, but in others the distinction is crucial.

The difference between BFS and DFS results is in the order in which they explore vertices. This order depends completely upon the container data structure used to store the *discovered* but not *processed* vertices.

- *Queue* – By storing the vertices in a first-in, first-out (FIFO) queue, we explore the oldest unexplored vertices first. Thus our explorations radiate out slowly from the starting vertex, defining a breadth-first search.

- *Stack* – By storing the vertices in a last-in, first-out (LIFO) stack, we explore the vertices by lurching along a path, visiting a new neighbor if one is available, and backing up only when we are surrounded by previously discovered vertices. Thus, our explorations quickly wander away from our starting point, defining a depth-first search.

Our implementation of `dfs` maintains a notion of traversal *time* for each vertex. Our `time` clock ticks each time we enter or exit any vertex. We keep track of the *entry* and *exit* times for each vertex.

Depth-first search has a neat recursive implementation, which eliminates the need to explicitly use a stack:

DFS(G, u)
    $state[u]$ = "discovered"
    process vertex u if desired
    $entry[u] = time$

$time = time + 1$
for each $v \in Adj[u]$ do
    process edge (u, v) if desired
    if $state[v]$ = "undiscovered" then
        $p[v] = u$
        DFS(G, v)
$state[u]$ = "processed"
$exit[u] = time$
$time = time + 1$

The time intervals have interesting and useful properties with respect to depth-first search:

- *Who is an ancestor?* – Suppose that x is an ancestor of y in the DFS tree. This implies that we must enter x before y, since there is no way we can be born before our own father or grandfather! We also must exit y before we exit x, because the mechanics of DFS ensure we cannot exit x until after we have backed up from the search of all its descendants. Thus the time interval of y must be properly nested within ancestor x.

- *How many descendants?* – The difference between the exit and entry times for v tells us how many descendents v has in the DFS tree. The clock gets incremented on each vertex entry and vertex exit, so half the time difference denotes the number of descendents of v.

We will use these entry and exit times in several applications of depth-first search, particularly topological sorting and biconnected/strongly-connected components. We need to be able to take separate actions on each entry and exit, thus motivating distinct `process_vertex_early` and `process_vertex_late` routines called from `dfs`.

The other important property of a depth-first search is that it partitions the edges of an undirected graph into exactly two classes: *tree edges* and *back edges*. The tree edges discover new vertices, and are those encoded in the `parent` relation. Back edges are those whose other endpoint is an ancestor of the vertex being expanded, so they point back into the tree.

An amazing property of depth-first search is that all edges fall into these two classes. Why can't an edge go to a brother or cousin node instead of an ancestor? All nodes reachable from a given vertex v are expanded before we finish with the traversal from v, so such topologies are impossible for undirected graphs. This edge classification proves fundamental to the correctness of DFS-based algorithms.

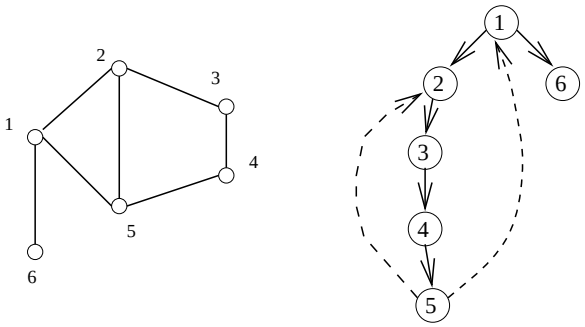


Figure 5.10: An undirected graph and its depth-first search tree

Implementation

A depth-first search can be thought of as a breadth-first search with a stack instead of a queue. The beauty of implementing `dfs` recursively is that recursion eliminates the need to keep an explicit stack:

```
dfs(graph *g, int v)
{
        edgenode *p;              /* temporary pointer */
        int y;                    /* successor vertex */

        if (finished) return;     /* allow for search termination */

        discovered[v] = TRUE;
        time = time + 1;
        entry_time[v] = time;

        process_vertex_early(v);

        p = g->edges[v];
        while (p != NULL) {
                y = p->y;
                if (discovered[y] == FALSE) {
                        parent[y] = v;
                        process_edge(v,y);
                        dfs(g,y);
                }
                else if ((!processed[y]) || (g->directed))
                        process_edge(v,y);
```

```
            if (finished) return;

            p = p->next;
        }

        process_vertex_late(v);

        time = time + 1;
        exit_time[v] = time;

        processed[v] = TRUE;
}
```

Depth-first search use essentially the same idea as backtracking, which we study in Section 7.1 (page 231). Both involve exhaustively searching all possibilities by advancing if it is possible, and backing up as soon as there is no unexplored possibility for further advancement. Both are most easily understood as recursive algorithms.

Take-Home Lesson: DFS organizes vertices by entry/exit times, and edges into tree and back edges. This organization is what gives DFS its real power.

5.9 Applications of Depth-First Search

As algorithm design paradigms go, a depth-first search isn't particularly intimidating. It is surprisingly *subtle*, however meaning that its correctness requires getting details right.

The correctness of a DFS-based algorithm depends upon specifics of exactly *when* we process the edges and vertices. We can process vertex v either before we have traversed any of the outgoing edges from v (`process_vertex_early()`) or after we have finished processing all of them (`process_vertex_late()`). Sometimes we will take special actions at both times, say `process_vertex_early()` to initialize a vertex-specific data structure, which will be modified on edge-processing operations and then analyzed afterwards using `process_vertex_late()`.

In undirected graphs, each edge (x, y) sits in the adjacency lists of vertex x and y. Thus there are two potential times to process each edge (x, y), namely when exploring x and when exploring y. The labeling of edges as tree edges or back edges occurs during the first time the edge is explored. This first time we see an edge is usually a logical time to do edge-specific processing. Sometimes, we may want to take different action the second time we see an edge.

But when we encounter edge (x, y) from x, how can we tell if we have previously traversed the edge from y? The issue is easy if vertex y is undiscovered: (x, y)

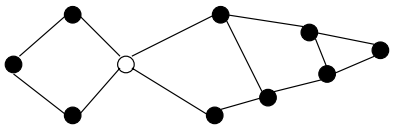


Figure 5.11: An articulation vertex is the weakest point in the graph

becomes a tree edge so this must be the first time. The issue is also easy if y has not been completely processed; since we explored the edge when we explored y this must be the second time. But what if y is an ancestor of x, and thus in a discovered state? Careful reflection will convince you that this must be our first traversal *unless* y is the immediate ancestor of x—i.e. , (y, x) is a tree edge. This can be established by testing if `y == parent[x]`.

I find that the subtlety of depth-first search-based algorithms kicks me in the head whenever I try to implement one. I encourage you to analyze these implementations carefully to see where the problematic cases arise and why.

5.9.1 Finding Cycles

Back edges are the key to finding a cycle in an undirected graph. If there is no back edge, all edges are tree edges, and no cycle exists in a tree. But *any* back edge going from x to an ancestor y creates a cycle with the tree path from y to x. Such a cycle is easy to find using `dfs`:

```
process_edge(int x, int y)
{
        if (parent[x] != y) {   /* found back edge! */
                printf("Cycle from %d to %d:",y,x);
                find_path(y,x,parent);
                printf("\n\n");
                finished = TRUE;
        }
}
```

The correctness of this cycle detection algorithm depends upon processing each undirected edge exactly once. Otherwise, a spurious two-vertex cycle (x, y, x) could be composed from the two traversals of any single undirected edge. We use the `finished` flag to terminate after finding the first cycle.

5.9.2 Articulation Vertices

Suppose you are a vandal seeking to disrupt the telephone network. Which station in Figure 5.11 should you choose to blow up to cause the maximum amount of

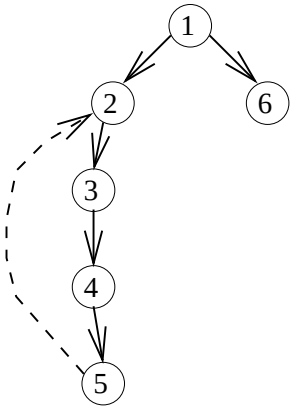


Figure 5.12: DFS tree of a graph containing two articulation vertices (namely 1 and 2). Back edge $(5, 2)$ keeps vertices 3 and 4 from being cut-nodes. Vertices 5 and 6 escape as leaves of the DFS tree

damage? Observe that there is a single point of failure—a single vertex whose deletion disconnects a connected component of the graph. Such a vertex is called an *articulation vertex* or *cut-node*. Any graph that contains an articulation vertex is inherently fragile, because deleting that single vertex causes a loss of connectivity between other nodes.

We presented a breadth-first search-based connected components algorithm in Section 5.7.1 (page 166). In general, the *connectivity* of a graph is the smallest number of vertices whose deletion will disconnect the graph. The connectivity is one if the graph has an articulation vertex. More robust graphs without such a vertex are said to be *biconnected*. Connectivity will be further discussed in the catalog in Section 15.8 (page 505).

Testing for articulation vertices by brute force is easy. Temporarily delete each vertex v, and then do a BFS or DFS traversal of the remaining graph to establish whether it is still connected. The total time for n such traversals is $O(n(m+n))$. There is a clever linear-time algorithm, however, that tests all the vertices of a connected graph using a single depth-first search.

What might the depth-first search tree tell us about articulation vertices? This tree connects all the vertices of the graph. If the DFS tree represented the entirety of the graph, all internal (nonleaf) nodes would be articulation vertices, since deleting any one of them would separate a leaf from the root. Blowing up a leaf (such as vertices 2 and 6 in Figure 5.12) cannot disconnect the tree, since it connects no one but itself to the main trunk.

The root of the search tree is a special case. If it has only one child, it functions as a leaf. But if the root has two or more children, its deletion disconnects them, making the root an articulation vertex.

General graphs are more complex than trees. But a depth-first search of a general graph partitions the edges into tree edges and back edges. Think of these back edges as security cables linking a vertex back to one of its ancestors. The security cable from x back to y ensures that none of the vertices on the tree path between x and y can be articulation vertices. Delete any of these vertices, and the security cable will still hold all of them to the rest of the tree.

Finding articulation vertices requires maintaining the extent to which back edges (i.e. , security cables) link chunks of the DFS tree back to ancestor nodes. Let `reachable_ancestor[v]` denote the earliest reachable ancestor of vertex v, meaning the oldest ancestor of v that we can reach by a combination of tree edges and back edges. Initially, `reachable_ancestor[v] = v`:

```
int reachable_ancestor[MAXV+1]; /* earliest reachable ancestor of v */
int tree_out_degree[MAXV+1];   /* DFS tree outdegree of v */

process_vertex_early(int v)
{
        reachable_ancestor[v] = v;
}
```

We update `reachable_ancestor[v]` whenever we encounter a back edge that takes us to an earlier ancestor than we have previously seen. The relative age/rank of our ancestors can be determined from their `entry_time`'s:

```
process_edge(int x, int y)
{
    int class;              /* edge class */

    class = edge_classification(x,y);

    if (class == TREE)
           tree_out_degree[x] = tree_out_degree[x] + 1;

    if ((class == BACK) && (parent[x] != y)) {
           if (entry_time[y] < entry_time[ reachable_ancestor[x] ] )
                    reachable_ancestor[x] = y;
     }
}
```

The key issue is determining how the reachability relation impacts whether vertex v is an articulation vertex. There are three cases, as shown in Figure 5.13:

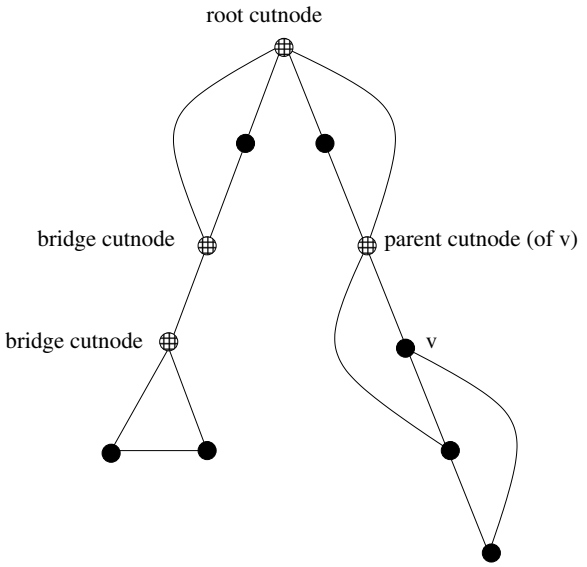


Figure 5.13: The three cases of articulation vertices: root, bridge, and parent cut-nodes

- *Root cut-nodes* – If the root of the DFS tree has two or more children, it must be an articulation vertex. No edges from the subtree of the second child can possibly connect to the subtree of the first child.

- *Bridge cut-nodes* – If the earliest reachable vertex from v is v, then deleting the single edge $(parent[v], v)$ disconnects the graph. Clearly $parent[v]$ must be an articulation vertex, since it cuts v from the graph. Vertex v is also an articulation vertex unless it is a leaf of the DFS tree. For any leaf, nothing falls off when you cut it.

- *Parent cut-nodes* – If the earliest reachable vertex from v is the parent of v, then deleting the parent must sever v from the tree unless the parent is the root.

The routine below systematically evaluates each of the three conditions as we back up from the vertex after traversing all outgoing edges. We use `entry_time[v]` to represent the age of vertex v. The reachability time `time_v` calculated below denotes the oldest vertex that can be reached using back edges. Getting back to an ancestor above v rules out the possibility of v being a cut-node:

```
process_vertex_late(int v)
{
     bool root;          /* is the vertex the root of the DFS tree? */
     int time_v;         /* earliest reachable time for v */
     int time_parent;    /* earliest reachable time for parent[v] */

     if (parent[v] < 1) {    /* test if v is the root */
             if (tree_out_degree[v] > 1)
                     printf("root articulation vertex: %d \n",v);
             return;
     }

     root = (parent[parent[v]] < 1);      /* is parent[v] the root? */
     if ((reachable_ancestor[v] == parent[v]) && (!root))
             printf("parent articulation vertex: %d \n",parent[v]);

     if (reachable_ancestor[v] == v) {
             printf("bridge articulation vertex: %d \n",parent[v]);

             if (tree_out_degree[v] > 0)  /* test if v is not a leaf */
                     printf("bridge articulation vertex: %d \n",v);
     }

     time_v = entry_time[reachable_ancestor[v]];
     time_parent = entry_time[ reachable_ancestor[parent[v]] ];

     if (time_v < time_parent)
             reachable_ancestor[parent[v]] = reachable_ancestor[v];
}
```

The last lines of this routine govern when we back up a node's highest reachable ancestor to its parent, namely whenever it is higher than the parent's earliest ancestor to date.

We can alternately talk about reliability in terms of edge failures instead of vertex failures. Perhaps our vandal would find it easier to cut a cable instead of blowing up a switching station. A single edge whose deletion disconnects the graph is called a *bridge*; any graph without such an edge is said to be *edge-biconnected*.

Identifying whether a given edge (x, y) is a bridge is easily done in linear time by deleting the edge and testing whether the resulting graph is connected. In fact all bridges can be identified in the same $O(n+m)$ time. Edge (x, y) is a bridge if (1) it is a tree edge, and (2) no back edge connects from y or below to x or above. This can be computed with a minor modification of the `reachable_ancestor` function.

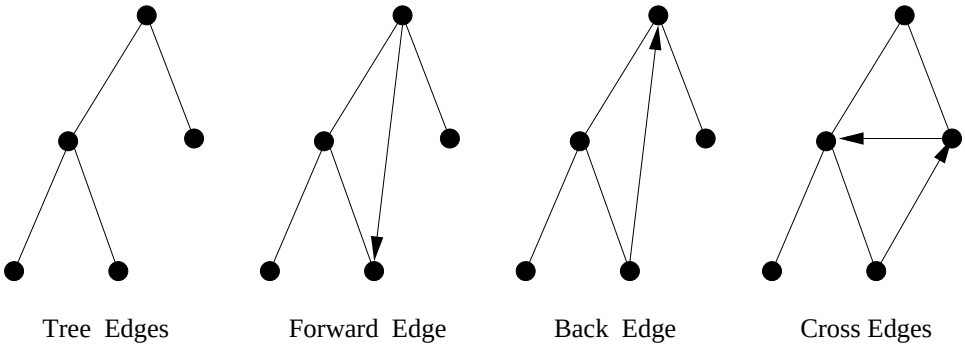


Figure 5.14: Possible edge cases for BFS/DFS traversal

5.10 Depth-First Search on Directed Graphs

Depth-first search on an undirected graph proves useful because it organizes the edges of the graph in a very precise way, as shown in Figure 5.10.

When traversing undirected graphs, every edge is either in the depth-first search tree or a back edge to an ancestor in the tree. Let us review why. Suppose we encountered a "forward edge" (x, y) directed toward a descendant vertex. In this case, we would have discovered (x, y) while exploring y, making it a back edge. Suppose we encounter a "cross edge" (x, y), linking two unrelated vertices. Again, we would have discovered this edge when we explored y, making it a tree edge.

For directed graphs, depth-first search labelings can take on a wider range of possibilities. Indeed, all four of the edge cases in Figure 5.14 can occur in traversing directed graphs. Still, this classification proves useful in organizing algorithms on directed graphs. We typically take a different action on edges from each different case.

The correct labeling of each edge can be readily determined from the state, discovery time, and parent of each vertex, as encoded in the following function:

```
int edge_classification(int x, int y)
{
 if (parent[y] == x) return(TREE);
 if (discovered[y] && !processed[y]) return(BACK);
 if (processed[y] && (entry_time[y]>entry_time[x])) return(FORWARD);
 if (processed[y] && (entry_time[y]<entry_time[x])) return(CROSS);

 printf("Warning: unclassified edge (%d,%d)\n",x,y);
}
```

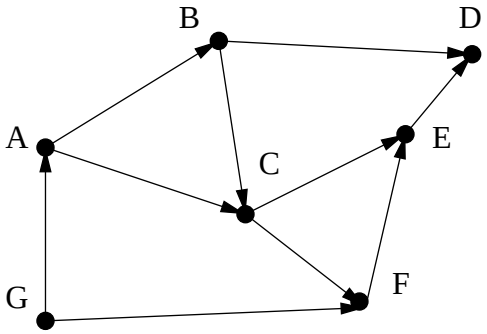


Figure 5.15: A DAG with only one topological sort (G, A, B, C, F, E, D)

As with BFS, this implementation of the depth-first search algorithm includes places to optionally process each vertex and edge—say to copy them, print them, or count them. Both algorithms will traverse all edges in the same connected component as the starting point. Since we need to start with a vertex in each component to traverse a disconnected graph, we must start from any vertex remaining undiscovered after a component search. With the proper initialization, this completes the traversal algorithm:

```
DFS-graph(G)
    for each vertex u ∈ V[G] do
        state[u] = "undiscovered"
            for each vertex u ∈ V[G] do
        if state[u] = "undiscovered" then
            initialize new component, if desired
            DFS(G, u)
```

I encourage the reader to convince themselves of the correctness of these four conditions. What I said earlier about the subtlety of depth-first search goes double for directed graphs.

5.10.1 Topological Sorting

Topological sorting is the most important operation on directed acyclic graphs (DAGs). It orders the vertices on a line such that all directed edges go from left to right. Such an ordering cannot exist if the graph contains a directed cycle, because there is no way you can keep going right on a line and still return back to where you started from!

Each DAG has at least one topological sort. The importance of topological sorting is that it gives us an ordering to process each vertex before any of its successors. Suppose the edges represented precedence constraints, such that edge

(x, y) means job x must be done before job y. Then, any topological sort defines a legal schedule. Indeed, there can be many such orderings for a given DAG.

But the applications go deeper. Suppose we seek the shortest (or longest) path from x to y in a DAG. No vertex appearing after y in the topological order can contribute to any such path, because there will be no way to get back to y. We can appropriately process all the vertices from left to right in topological order, considering the impact of their outgoing edges, and know that we will have looked at everything we need before we need it. Topological sorting proves very useful in essentially any algorithmic problem on directed graphs, as discussed in the catalog in Section 15.2 (page 481).

Topological sorting can be performed efficiently using depth-first searching. A directed graph is a DAG if and only if no back edges are encountered. Labeling the vertices in the reverse order that they are marked *processed* finds a topological sort of a DAG. Why? Consider what happens to each directed edge $\{x, y\}$ as we encounter it exploring vertex x:

- If y is currently *undiscovered*, then we start a DFS of y before we can continue with x. Thus y is marked *completed* before x is, and x appears before y in the topological order, as it must.
- If y is *discovered* but not *completed*, then $\{x, y\}$ is a back edge, which is forbidden in a DAG.
- If y is *processed*, then it will have been so labeled before x. Therefore, x appears before y in the topological order, as it must.

Study the following implementation:

```
process_vertex_late(int v)
{
        push(&sorted,v);
}


process_edge(int x, int y)
{
        int class;              /* edge class */

        class = edge_classification(x,y);

        if (class == BACK)
               printf("Warning: directed cycle found, not a DAG\n");
}
```

```
topsort(graph *g)
{
        int i;                          /* counter */

        init_stack(&sorted);

        for (i=1; i<=g->nvertices; i++)
                if (discovered[i] == FALSE)
                        dfs(g,i);

        print_stack(&sorted);           /* report topological order */
}
```

We push each vertex on a stack as soon as we have evaluated all outgoing edges. The top vertex on the stack always has no incoming edges from any vertex on the stack. Repeatedly popping them off yields a topological ordering.

5.10.2 Strongly Connected Components

We are often concerned with *strongly connected components*—that is, partitioning a graph into chunks such that directed paths exist between all pairs of vertices within a given chunk. A directed graph is *strongly connected* if there is a directed path between any two vertices. Road networks should be strongly connected, or else there will be places you can drive to but not drive home from without violating one-way signs.

It is straightforward to use graph traversal to test whether a graph $G = (V, E)$ is strongly connected in linear time. First, do a traversal from some arbitrary vertex v. Every vertex in the graph had better be reachable from v (and hence discovered on the BFS or DFS starting from v), otherwise G cannot possibly be strongly connected. Now construct a graph $G' = (V, E')$ with the same vertex and edge set as G but with all edges reversed—i.e., directed edge $(x, y) \in E$ iff $(y, x) \in E'$. Thus, any path from v to z in G' corresponds to a path from z to v in G. By doing a DFS from v in G', we find all vertices with paths *to* v in G. The graph is strongly connected iff all vertices in G can (1) reach v and (2) are reachable from v.

Graphs that are not strongly connected can be partitioned into strongly connected components, as shown in Figure 5.16 (left). The set of such components and the weakly-connecting edges that link them together can be determined using DFS. The algorithm is based on the observation that it is easy to find a directed cycle using a depth-first search, since any back edge plus the down path in the DFS tree gives such a cycle. All vertices in this cycle must be in the same strongly connected component. Thus, we can shrink (contract) the vertices on this cycle down to a single vertex representing the component, and then repeat. This process terminates when no directed cycle remains, and each vertex represents a different strongly connected component.

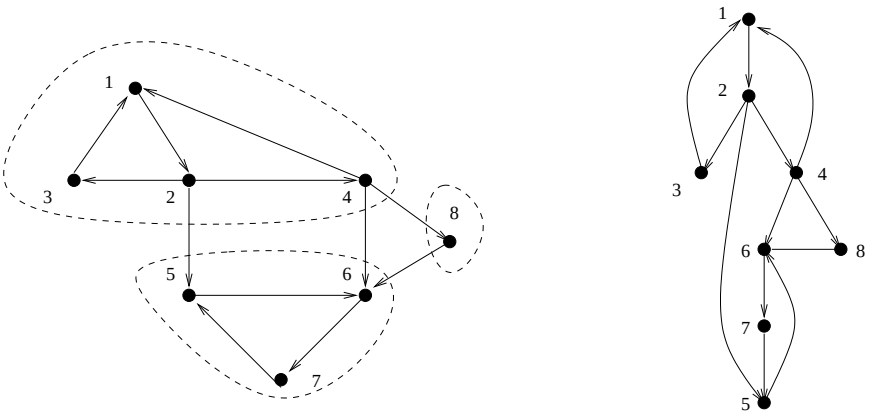


Figure 5.16: The strongly-connected components of a graph, with the associated DFS tree

Our approach to implementing this idea is reminiscent of finding biconnected components in Section 5.9.2 (page 173). We update our notion of the oldest reachable vertex in response to (1) nontree edges and (2) backing up from a vertex. Because we are working on a directed graph, we also must contend with forward edges (from a vertex to a descendant) and cross edges (from a vertex back to an nonancestor but previously discovered vertex). Our algorithm will peal one strong component off the tree at a time, and assign each of its vertices the number of the component it is in:

```
strong_components(graph *g)
{
        int i;                          /* counter */

        for (i=1; i<=(g->nvertices); i++) {
                low[i] = i;
                scc[i] = -1;
        }
        components_found = 0;
        init_stack(&active);
        initialize_search(&g);

        for (i=1; i<=(g->nvertices); i++)
                if (discovered[i] == FALSE) {
                        dfs(g,i);
                }
}
```

Define `low[v]` to be the oldest vertex known to be in the same strongly connected component as v. This vertex is not necessarily an ancestor, but may also be a distant cousin of v because of cross edges. Cross edges that point vertices from *previous* strongly connected components of the graph cannot help us, because there can be no way back from them to v, but otherwise cross edges are fair game. Forward edges have no impact on reachability over the depth-first tree edges, and hence can be disregarded:

```
int low[MAXV+1];        /* oldest vertex surely in component of v */
int scc[MAXV+1];        /* strong component number for each vertex */


process_edge(int x, int y)
{
        int class;           /* edge class */

        class = edge_classification(x,y);

        if (class == BACK) {
                if (entry_time[y] < entry_time[ low[x] ] )
                        low[x] = y;
        }

        if (class == CROSS) {
                if (scc[y] == -1)  /* component not yet assigned */
                        if (entry_time[y] < entry_time[ low[x] ] )
                                low[x] = y;
        }
}
```

A new strongly connected component is found whenever the lowest reachable vertex from v is v. If so, we can clear the stack of this component. Otherwise, we give our parent the benefit of the oldest ancestor we can reach and backtrack:

```
process_vertex_early(int v)
{
        push(&active,v);
}
```

```
process_vertex_late(int v)
{
      if (low[v] == v) {     /* edge (parent[v],v) cuts off scc */
              pop_component(v);
      }

      if (entry_time[low[v]] < entry_time[low[parent[v]]])
              low[parent[v]] = low[v];
}


pop_component(int v)
{
      int t;                /* vertex placeholder */

      components_found = components_found + 1;

      scc[ v ] = components_found;
      while ((t = pop(&active)) != v) {
              scc[ t ] = components_found;
      }
}
```

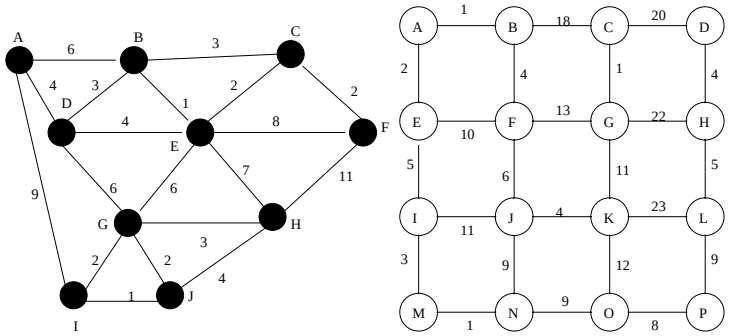
Chapter Notes

Our treatment of graph traversal represents an expanded version of material from Chapter 9 of [SR03]. The *Combinatorica* graph library discussed in the war story is best described in the old [Ski90]. and new editions [PS03] of the associated book. Accessible introductions to the science of social networks include Barabasi [Bar03] and Watts [Wat04].

5.11 Exercises

Simulating Graph Algorithms

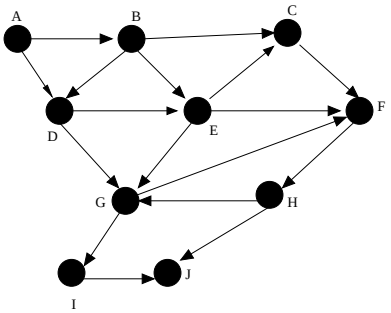
5-1. *[3]* For the following graphs G_1 (left) and G_2 (right):



(a) Report the order of the vertices encountered on a breadth-first search starting from vertex A. Break all ties by picking the vertices in alphabetical order (i.e., A before Z).

(b) Report the order of the vertices encountered on a depth-first search starting from vertex A. Break all ties by picking the vertices in alphabetical order (i.e., A before Z).

5-2. *[3]* Do a topological sort of the following graph G:



Traversal

5-3. *[3]* Prove by induction that there is a unique path between any pair of vertices in a tree.

5-4. *[3]* Prove that in a breadth-first search on a undirected graph G, every edge is either a tree edge or a cross edge, where x is neither an ancestor nor descendant of y, in cross edge (x, y).

5-5. *[3]* Give a linear algorithm to compute the chromatic number of graphs where each vertex has degree at most 2. Must such graphs be bipartite?

5-6. *[5]* In breadth-first and depth-first search, an undiscovered node is marked *discovered* when it is first encountered, and marked *processed* when it has been completely

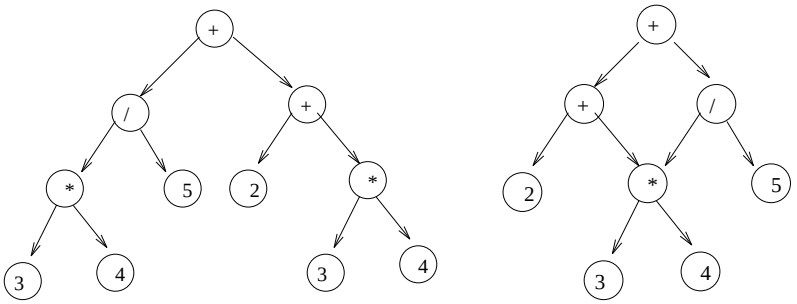


Figure 5.17: Expression $2 + 3 * 4 + (3 * 4)/5$ as a tree and a DAG

searched. At any given moment, several nodes might be simultaneously in the *discovered* state.

(a) Describe a graph on n vertices and a particular starting vertex v such that $\Theta(n)$ nodes are simultaneously in the *discovered* state during a *breadth-first search* starting from v.

(b) Describe a graph on n vertices and a particular starting vertex v such that $\Theta(n)$ nodes are simultaneously in the *discovered* state during a *depth-first search* starting from v.

(c) Describe a graph on n vertices and a particular starting vertex v such that at some point $\Theta(n)$ nodes remain *undiscovered*, while $\Theta(n)$ nodes have been *processed* during a *depth-first search* starting from v. (Note, there may also be *discovered* nodes.)

5-7. *[4]* Given pre-order and in-order traversals of a binary tree, is it possible to reconstruct the tree? If so, sketch an algorithm to do it. If not, give a counterexample. Repeat the problem if you are given the pre-order and post-order traversals.

5-8. *[3]* Present correct and efficient algorithms to convert an undirected graph G between the following graph data structures. You must give the time complexity of each algorithm, assuming n vertices and m edges.

(a) Convert from an adjacency matrix to adjacency lists.

(b) Convert from an adjacency list to an incidence matrix. An incidence matrix M has a row for each vertex and a column for each edge, such that $M[i, j] = 1$ if vertex i is part of edge j, otherwise $M[i, j] = 0$.

(c) Convert from an incidence matrix to adjacency lists.

5-9. *[3]* Suppose an arithmetic expression is given as a tree. Each leaf is an integer and each internal node is one of the standard arithmetical operations $(+, -, *, /)$. For example, the expression $2 + 3 * 4 + (3 * 4)/5$ is represented by the tree in Figure 5.17(a). Give an $O(n)$ algorithm for evaluating such an expression, where there are n nodes in the tree.

5-10. *[5]* Suppose an arithmetic expression is given as a DAG (directed acyclic graph) with common subexpressions removed. Each leaf is an integer and each internal

node is one of the standard arithmetical operations $(+, -, *, /)$. For example, the expression $2 + 3 * 4 + (3 * 4)/5$ is represented by the DAG in Figure 5.17(b). Give an $O(n + m)$ algorithm for evaluating such a DAG, where there are n nodes and m edges in the DAG. Hint: modify an algorithm for the tree case to achieve the desired efficiency.

5-11. *[8]* The war story of Section 5.4 (page 158) describes an algorithm for constructing the dual graph of the triangulation efficiently, although it does not guarantee linear time. Give a worst-case linear algorithm for the problem.

Algorithm Design

5-12. *[5]* The *square* of a directed graph $G = (V, E)$ is the graph $G^2 = (V, E^2)$ such that $(u, w) \in E^2$ iff there exists $v \in V$ such that $(u, v) \in E$ and $(v, w) \in E$; i.e., there is a path of exactly two edges from u to w.

Give efficient algorithms for both adjacency lists and matrices.

5-13. *[5]* A *vertex cover* of a graph $G = (V, E)$ is a subset of vertices V' such that each edge in E is incident on at least one vertex of V'.

(a) Give an efficient algorithm to find a minimum-size vertex cover if G is a tree.

(b) Let $G = (V, E)$ be a tree such that the weight of each vertex is equal to the degree of that vertex. Give an efficient algorithm to find a minimum-weight vertex cover of G.

(c) Let $G = (V, E)$ be a tree with arbitrary weights associated with the vertices. Give an efficient algorithm to find a minimum-weight vertex cover of G.

5-14. *[3]* A *vertex cover* of a graph $G = (V, E)$ is a subset of vertices $V' \in V$ such that every edge in E contains at least one vertex from V'. Delete all the leaves from any depth-first search tree of G. Must the remaining vertices form a vertex cover of G? Give a proof or a counterexample.

5-15. *[5]* A *vertex cover* of a graph $G = (V, E)$ is a subset of vertices $V' \in V$ such that every edge in E contains *at least one* vertex from V'. An *independent set* of graph $G = (V, E)$ is a subset of vertices $V' \in V$ such that no edge in E contains both vertices from V'.

An *independent vertex cover* is a subset of vertices that is both an independent set and a vertex cover of G. Give an efficient algorithm for testing whether G contains an independent vertex cover. What classical graph problem does this reduce to?

5-16. *[5]* An *independent set* of an undirected graph $G = (V, E)$ is a set of vertices U such that no edge in E is incident on two vertices of U.

(a) Give an efficient algorithm to find a maximum-size independent set if G is a tree.

(b) Let $G = (V, E)$ be a tree with weights associated with the vertices such that the weight of each vertex is equal to the degree of that vertex. Give an efficient algorithm to find a maximum independent set of G.

(c) Let $G = (V, E)$ be a tree with arbitrary weights associated with the vertices. Give an efficient algorithm to find a maximum independent set of G.

5-17. *[5]* Consider the problem of determining whether a given undirected graph $G = (V, E)$ contains a *triangle* or cycle of length 3.

(a) Give an $O(|V|^3)$ to find a triangle if one exists.

(b) Improve your algorithm to run in time $O(|V| \cdot |E|)$. You may assume $|V| \leq |E|$.

Observe that these bounds gives you time to convert between the adjacency matrix and adjacency list representations of G.

5-18. *[5]* Consider a set of movies $M_1, M_2, \ldots, M_k$. There is a set of customers, each one of which indicates the two movies they would like to see this weekend. Movies are shown on Saturday evening and Sunday evening. Multiple movies may be screened at the same time.

You must decide which movies should be televised on Saturday and which on Sunday, so that every customer gets to see the two movies they desire. Is there a schedule where each movie is shown at most once? Design an efficient algorithm to find such a schedule if one exists.

5-19. *[5]* The *diameter* of a tree $T = (V, E)$ is given by

$$\max_{u,v \in V} \delta(u, v)$$

(where $\delta(u, v)$ is the number of edges on the path from u to v). Describe an efficient algorithm to compute the diameter of a tree, and show the correctness and analyze the running time of your algorithm.

5-20. *[5]* Given an undirected graph G with n vertices and m edges, and an integer k, give an $O(m + n)$ algorithm that finds the maximum induced subgraph H of G such that each vertex in H has degree $\geq k$, or prove that no such graph exists. An induced subgraph $F = (U, R)$ of a graph $G = (V, E)$ is a subset of U of the vertices V of G, and all edges R of G such that both vertices of each edge are in U.

5-21. *[6]* Let v and w be two vertices in a directed graph $G = (V, E)$. Design a linear-time algorithm to find the *number* of different shortest paths (not necessarily vertex disjoint) between v and w. Note: the edges in G are unweighted.

5-22. *[6]* Design a linear-time algorithm to eliminate each vertex v of degree 2 from a graph by replacing edges (u, v) and (v, w) by an edge (u, w). We also seek to eliminate multiple copies of edges by replacing them with a single edge. Note that removing multiple copies of an edge may create a new vertex of degree 2, which has to be removed, and that removing a vertex of degree 2 may create multiple edges, which also must be removed.

Directed Graphs

5-23. *[5]* Your job is to arrange n ill-behaved children in a straight line, facing front. You are given a list of m statements of the form "i hates j". If i hates j, then you do not want put i somewhere behind j, because then i is capable of throwing something at j.

(a) Give an algorithm that orders the line, (or says that it is not possible) in $O(m + n)$ time.

(b) Suppose instead you want to arrange the children in rows such that if i hates j, then i must be in a lower numbered row than j. Give an efficient algorithm to find the minimum number of rows needed, if it is possible.

5-24. *[3]* Adding a single directed edge to a directed graph can reduce the number of weakly connected components, but by at most how many components? What about the number of strongly connected components?

5-25. *[5]* An *arborescence* of a directed graph G is a rooted tree such that there is a directed path from the root to every other vertex in the graph. Give an efficient and correct algorithm to test whether G contains an arborescence, and its time complexity.

5-26. *[5]* A *mother* vertex in a directed graph $G = (V, E)$ is a vertex v such that all other vertices G can be reached by a directed path from v.

(a) Give an $O(n + m)$ algorithm to test whether a given vertex v is a mother of G, where $n = |V|$ and $m = |E|$.

(b) Give an $O(n+m)$ algorithm to test whether graph G contains a mother vertex.

5-27. *[9]* A *tournament* is a directed graph formed by taking the complete undirected graph and assigning arbitrary directions on the edges—i.e., a graph $G = (V, E)$ such that for all u,$v \in V$, exactly one of (u, v) or (v, u) is in E. Show that every tournament has a Hamiltonian path—that is, a path that visits every vertex exactly once. Give an algorithm to find this path.

Articulation Vertices

5-28. *[5]* An articulation vertex of a graph G is a vertex whose deletion disconnects G. Let G be a graph with n vertices and m edges. Give a simple $O(n + m)$ algorithm for finding a vertex of G that is *not* an articulation vertex—i.e. , whose deletion does not disconnect G.

5-29. *[5]* Following up on the previous problem, give an $O(n + m)$ algorithm that finds a deletion order for the n vertices such that no deletion disconnects the graph. (Hint: think DFS/BFS.)

5-30. *[3]* Suppose G is a connected undirected graph. An edge e whose removal disconnects the graph is called a *bridge*. Must every bridge e be an edge in a depth-first search tree of G? Give a proof or a counterexample.

Interview Problems

5-31. *[3]* Which data structures are used in depth-first and breath-first search?

5-32. *[4]* Write a function to traverse binary search tree and return the ith node in sorted order.

Programming Challenges

These programming challenge problems with robot judging are available at *http://www.programming-challenges.com* or *http://online-judge.uva.es*.

5-1. "Bicoloring" – Programming Challenges 110901, UVA Judge 10004.

5-2. "Playing with Wheels" – Programming Challenges 110902, UVA Judge 10067.

5-3. "The Tourist Guide" – Programming Challenges 110903, UVA Judge 10099.

5-4. "Edit Step Ladders" – Programming Challenges 110905, UVA Judge 10029.

5-5. "Tower of Cubes" – Programming Challenges 110906, UVA Judge 10051.

6

Weighted Graph Algorithms

The data structures and traversal algorithms of Chapter 5 provide the basic building blocks for any computation on graphs. However, all the algorithms presented there dealt with unweighted graphs—i.e. , graphs where each edge has identical value or weight.

There is an alternate universe of problems for *weighted graphs*. The edges of road networks are naturally bound to numerical values such as construction cost, traversal time, length, or speed limit. Identifying the shortest path in such graphs proves more complicated than breadth-first search in unweighted graphs, but opens the door to a wide range of applications.

The graph data structure from Chapter 5 quietly supported edge-weighted graphs, but here we make this explicit. Our adjacency list structure consists of an array of linked lists, such that the outgoing edges from vertex x appear in the list `edges[x]`:

```
typedef struct {
        edgenode *edges[MAXV+1];   /* adjacency info */
        int degree[MAXV+1];        /* outdegree of each vertex */
        int nvertices;             /* number of vertices in graph */
        int nedges;                /* number of edges in graph */
        int directed;              /* is the graph directed? */
} graph;
```

Each `edgenode` is a record containing three fields, the first describing the second endpoint of the edge (`y`), the second enabling us to annotate the edge with a weight (`weight`), and the third pointing to the next edge in the list (`next`):

S.S. Skiena, *The Algorithm Design Manual*, 2nd ed., DOI: 10.1007/978-1-84800-070-4_6,
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```
typedef struct {
        int y;                          /* adjacency info */
        int weight;                     /* edge weight, if any */
        struct edgenode *next;          /* next edge in list */
} edgenode;
```

We now describe several sophisticated algorithms using this data structure, including minimum spanning trees, shortest paths, and maximum flows. That these optimization problems can be solved efficiently is quite worthy of our respect. Recall that no such algorithm exists for the first weighted graph problem we encountered, namely the traveling salesman problem.

6.1 Minimum Spanning Trees

A *spanning tree* of a graph $G = (V, E)$ is a subset of edges from E forming a tree connecting all vertices of V. For edge-weighted graphs, we are particularly interested in the *minimum spanning tree*—the spanning tree whose sum of edge weights is as small as possible.

Minimum spanning trees are the answer whenever we need to connect a set of points (representing cities, homes, junctions, or other locations) by the smallest amount of roadway, wire, or pipe. Any tree is the smallest possible connected graph in terms of number of edges, while the minimum spanning tree is the smallest connected graph in terms of edge weight. In geometric problems, the point set $p_1, \ldots, p_n$ defines a complete graph, with edge (v_i, v_j) assigned a weight equal to the distance from p_i to p_j. An example of a geometric minimum spanning tree is illustrated in Figure 6.1. Additional applications of minimum spanning trees are discussed in Section 15.3 (page 484).

A minimum spanning tree minimizes the total length over all possible spanning trees. However, there can be more than one minimum spanning tree in a graph. Indeed, all spanning trees of an unweighted (or equally weighted) graph G are minimum spanning trees, since each contains exactly $n - 1$ equal-weight edges. Such a spanning tree can be found using depth-first or breadth-first search. Finding a minimum spanning tree is more difficult for general weighted graphs, however two different algorithms are presented below. Both demonstrate the optimality of certain greedy heuristics.

6.1.1 Prim's Algorithm

Prim's minimum spanning tree algorithm starts from one vertex and grows the rest of the tree one edge at a time until all vertices are included.

Greedy algorithms make the decision of what to do next by selecting the best local option from all available choices without regard to the global structure. Since we seek the tree of minimum weight, the natural greedy algorithm for minimum

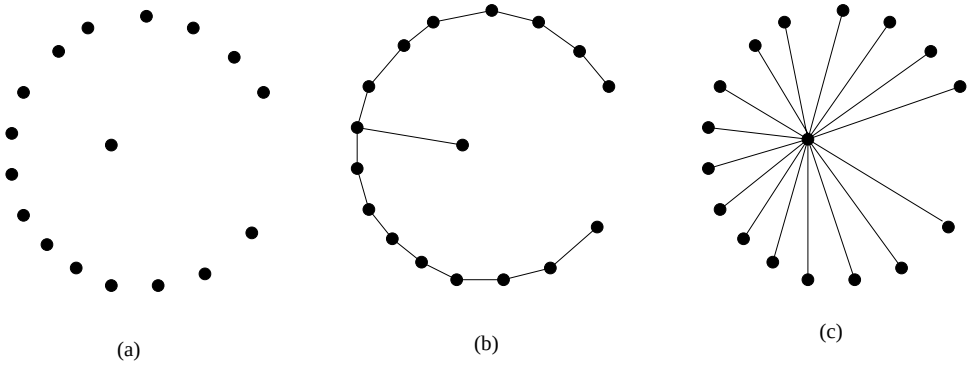

Figure 6.1: (a) Two spanning trees of point set; (b) the minimum spanning tree, and (c) the shortest path from center tree

---

spanning tree repeatedly selects the smallest weight edge that will enlarge the number of vertices in the tree.

Prim-MST(G)
    Select an arbitrary vertex s to start the tree from.
    While (there are still nontree vertices)
        Select the edge of minimum weight between a tree and nontree vertex
        Add the selected edge and vertex to the tree T_{prim}.

Prim's algorithm clearly creates a spanning tree, because no cycle can be introduced by adding edges between tree and nontree vertices. However, why should it be of minimum weight over all spanning trees? We have seen ample evidence of other natural greedy heuristics that do not yield a global optimum. Therefore, we must be particularly careful to demonstrate any such claim.

We use proof by contradiction. Suppose that there existed a graph G for which Prim's algorithm did not return a minimum spanning tree. Since we are building the tree incrementally, this means that there must have been some particular instant where we went wrong. Before we inserted edge (x, y), T_{prim} consisted of a set of edges that was a subtree of some minimum spanning tree T_{min}, but choosing edge (x, y) fatally took us away from a minimum spanning tree (see Figure 6.2(a)).

But how could we have gone wrong? There must be a path p from x to y in T_{min}, as shown in Figure 6.2(b). This path must use an edge (v_1, v_2), where v_1 is in T_{prim}, but v_2 is not. This edge (v_1, v_2) must have weight at least that of (x, y), or Prim's algorithm would have selected it before (x, y) when it had the chance. Inserting (x, y) and deleting (v_1, v_2) from T_{min} leaves a spanning tree no larger than before, meaning that Prim's algorithm did not make a fatal mistake in selecting edge (x, y). Therefore, by contradiction, Prim's algorithm must construct a minimum spanning tree.

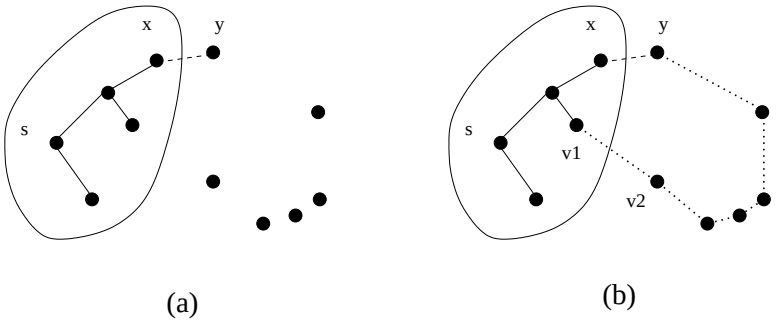

Figure 6.2: Where Prim's algorithm goes bad? No, because $d(v_1, v_2) \geq d(x, y)$

Implementation

Prim's algorithm grows the minimum spanning tree in stages, starting from a given vertex. At each iteration, we add one new vertex into the spanning tree. A greedy algorithm suffices for correctness: we always add the lowest-weight edge linking a vertex in the tree to a vertex on the outside. The simplest implementation of this idea would assign each vertex a Boolean variable denoting whether it is already in the tree (the array `intree` in the code below), and then searches all edges at each iteration to find the minimum weight edge with exactly one `intree` vertex.

Our implementation is somewhat smarter. It keeps track of the cheapest edge linking every nontree vertex in the tree. The cheapest such edge over all remaining non-tree vertices gets added in each iteration. We must update the costs of getting to the non-tree vertices after each insertion. However, since the most recently inserted vertex is the only change in the tree, all possible edge-weight updates must come from its outgoing edges:

```
prim(graph *g, int start)
{
    int i;                      /* counter */
    edgenode *p;                /* temporary pointer */
    bool intree[MAXV+1];        /* is the vertex in the tree yet? */
    int distance[MAXV+1];       /* cost of adding to tree */
    int v;                      /* current vertex to process */
    int w;                      /* candidate next vertex */
    int weight;                 /* edge weight */
    int dist;                   /* best current distance from start */

    for (i=1; i<=g->nvertices; i++) {
            intree[i] = FALSE;
```

```
            distance[i] = MAXINT;
            parent[i] = -1;
        }

    distance[start] = 0;
    v = start;

    while (intree[v] == FALSE) {
           intree[v] = TRUE;
           p = g->edges[v];
           while (p != NULL) {
                  w = p->y;
                  weight = p->weight;
                  if ((distance[w] > weight) && (intree[w] == FALSE)) {
                         distance[w] = weight;
                         parent[w] = v;
                    }
                    p = p->next;
            }

            v = 1;
            dist = MAXINT;
            for (i=1; i<=g->nvertices; i++)
                    if ((intree[i] == FALSE) && (dist > distance[i])) {
                            dist = distance[i];
                            v = i;
                    }
    }
}
```

Analysis

Prim's algorithm is correct, but how efficient is it? This depends on which data structures are used to implement it. In the pseudocode, Prim's algorithm makes n iterations sweeping through all m edges on each iteration—yielding an $O(mn)$ algorithm.

But our implementation avoids the need to test all m edges on each pass. It only considers the $\leq n$ cheapest known edges represented in the `parent` array and the $\leq n$ edges out of new tree vertex v to update `parent`. By maintaining a Boolean flag along with each vertex to denote whether it is in the tree or not, we test whether the current edge joins a tree with a non-tree vertex in constant time.

The result is an $O(n^2)$ implementation of Prim's algorithm, and a good illustration of power of data structures to speed up algorithms. In fact, more sophisticated

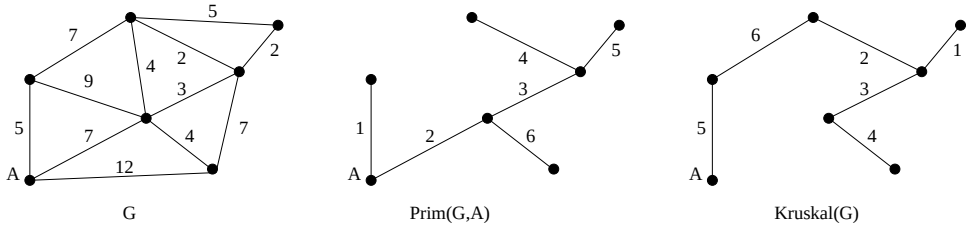

Figure 6.3: A graph G (l) with minimum spanning trees produced by Prim's (m) and Kruskal's (r) algorithms. The numbers on the trees denote the order of insertion; ties are broken arbitrarily

priority-queue data structures lead to an $O(m+n \lg n)$ implementation, by making it faster to find the minimum cost edge to expand the tree at each iteration.

The minimum spanning tree itself or its cost can be reconstructed in two different ways. The simplest method would be to augment this procedure with statements that print the edges as they are found or totals the weight of all selected edges. Alternately, the tree topology is encoded by the `parent` array, so it plus the original graph describe everything about the minimum spanning tree.

6.1.2 Kruskal's Algorithm

Kruskal's algorithm is an alternate approach to finding minimum spanning trees that proves more efficient on sparse graphs. Like Prim's, Kruskal's algorithm is greedy. Unlike Prim's, it does not start with a particular vertex.

Kruskal's algorithm builds up connected components of vertices, culminating in the minimum spanning tree. Initially, each vertex forms its own separate component in the tree-to-be. The algorithm repeatedly considers the lightest remaining edge and tests whether its two endpoints lie within the same connected component. If so, this edge will be discarded, because adding it would create a cycle in the tree-to-be. If the endpoints are in different components, we insert the edge and merge the two components into one. Since each connected component is always a tree, we need never explicitly test for cycles.

```
Kruskal-MST(G)
    Put the edges in a priority queue ordered by weight.
    count = 0
    while (count < n − 1) do
        get next edge (v, w)
        if (component (v) ≠ component(w))
            add to T_kruskal
            merge component(v) and component(w)
```

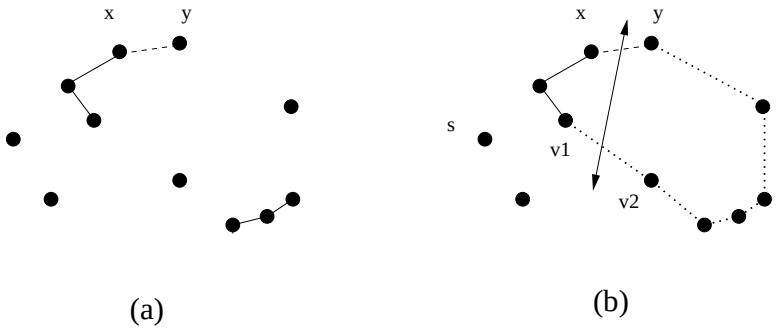

Figure 6.4: Where Kruskal's algorithm goes bad? No, because $d(v_1, v_2) \geq d(x, y)$

This algorithm adds $n-1$ edges without creating a cycle, so it clearly creates a spanning tree for any connected graph. But why must this be a *minimum* spanning tree? Suppose it wasn't. As with the correctness proof of Prim's algorithm, there must be some graph on which it fails. In particular, there must a single edge (x, y) whose insertion first prevented the tree $T_{kruskal}$ from being a minimum spanning tree T_{min}. Inserting this edge (x, y) into T_{min} will create a cycle with the path from x to y. Since x and y were in different components at the time of inserting (x, y), at least one edge (say (v_1, v_2)) on this path would have been evaluated by Kruskal's algorithm later than (x, y). But this means that $w(v_1, v_2) \geq w(x, y)$, so exchanging the two edges yields a tree of weight at most T_{min}. Therefore, we could not have made a fatal mistake in selecting (x, y), and the correctness follows.

What is the time complexity of Kruskal's algorithm? Sorting the m edges takes $O(m \lg m)$ time. The for loop makes m iterations, each testing the connectivity of two trees plus an edge. In the most simple-minded approach, this can be implemented by breadth-first or depth-first search in a sparse graph with at most n edges and n vertices, thus yielding an $O(mn)$ algorithm.

However, a faster implementation results if we can implement the component test in faster than $O(n)$ time. In fact, a clever data structure called *union-find*, can support such queries in $O(\lg n)$ time. Union-find is discussed in the next section. With this data structure, Kruskal's algorithm runs in $O(m \lg m)$ time, which is faster than Prim's for sparse graphs. Observe again the impact that the right data structure can have when implementing a straightforward algorithm.

Implementation

The implementation of the main routine follows fairly directly from the psuedocode:

```
kruskal(graph *g)
{
    int i;                      /* counter */
    set_union s;                /* set union data structure */
    edge_pair e[MAXV+1];        /* array of edges data structure */
    bool weight_compare();

    set_union_init(&s, g->nvertices);

    to_edge_array(g, e);        /* sort edges by increasing cost */
    qsort(&e,g->nedges,sizeof(edge_pair),weight_compare);

    for (i=0; i<(g->nedges); i++) {
            if (!same_component(s,e[i].x,e[i].y)) {
                    printf("edge (%d,%d) in MST\n",e[i].x,e[i].y);
                    union_sets(&s,e[i].x,e[i].y);
            }
    }
}
```

6.1.3 The Union-Find Data Structure

A *set partition* is a partitioning of the elements of some universal set (say the integers 1 to n) into a collection of disjointed subsets. Thus, each element must be in exactly one subset. Set partitions naturally arise in graph problems such as connected components (each vertex is in exactly one connected component) and vertex coloring (a person may be male or female, but not both or neither). Section 14.6 (page 456) presents algorithms for generating set partitions and related objects.

The connected components in a graph can be represented as a set partition. For Kruskal's algorithm to run efficiently, we need a data structure that efficiently supports the following operations:

- *Same component*(v_1, v_2) – Do vertices v_1 and v_2 occur in the same connected component of the current graph?
- *Merge components*(C_1, C_2) – Merge the given pair of connected components into one component in response to an edge between them.

The two obvious data structures for this task each support only one of these operations efficiently. Explicitly labeling each element with its component number enables the *same component* test to be performed in constant time, but updating the component numbers after a merger would require linear time. Alternately, we can treat the merge components operation as inserting an edge in a graph, but

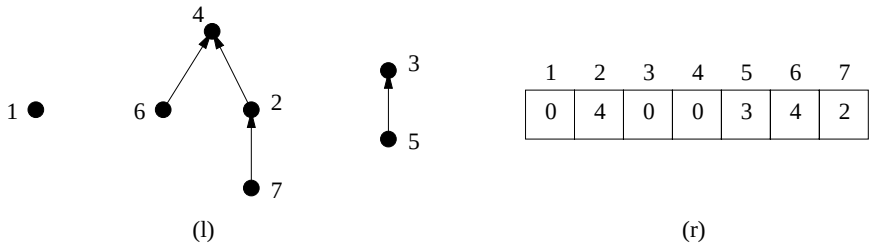

Figure 6.5: Union-find example: structure represented as trees (l) and array (r)

then we must run a full graph traversal to identify the connected components on demand.

The union-find data structure represents each subset as a "backwards" tree, with pointers from a node to its parent. Each node of this tree contains a set element, and the *name* of the set is taken from the key at the root. For reasons that will become clear, we will also maintain the number of elements in the subtree rooted in each vertex v:

```
typedef struct {
      int p[SET_SIZE+1];       /* parent element */
      int size[SET_SIZE+1];    /* number of elements in subtree i */
      int n;                   /* number of elements in set */
} set_union;
```

We implement our desired component operations in terms of two simpler operations, *union* and *find*:

- *Find(i)* – Find the root of tree containing element i, by walking up the parent pointers until there is nowhere to go. Return the label of the root.

- *Union(i,j)* – Link the root of one of the trees (say containing i) to the root of the tree containing the other (say j) so $find(i)$ now equals $find(j)$.

We seek to minimize the time it takes to execute *any* sequence of unions and finds. Tree structures can be very unbalanced, so we must limit the height of our trees. Our most obvious means of control is the decision of which of the two component roots becomes the root of the combined component on each *union*.

To minimize the tree height, it is better to make the smaller tree the subtree of the bigger one. Why? The height of all the nodes in the root subtree stay the same, while the height of the nodes merged into this tree all increase by one. Thus, merging in the smaller tree leaves the height unchanged on the larger set of vertices.

Implementation

The implementation details are as follows:

```
set_union_init(set_union *s, int n)
{
        int i;                          /* counter */

        for (i=1; i<=n; i++) {
                s->p[i] = i;
                s->size[i] = 1;
        }

        s->n = n;
}

int find(set_union *s, int x)
{
        if (s->p[x] == x)
                return(x);
        else
                return( find(s,s->p[x]) );
}

int union_sets(set_union *s, int s1, int s2)
{
        int r1, r2;                     /* roots of sets */

        r1 = find(s,s1);
        r2 = find(s,s2);

        if (r1 == r2) return;           /* already in same set */

        if (s->size[r1] >= s->size[r2]) {
                s->size[r1] = s->size[r1] + s->size[r2];
                s->p[ r2 ] = r1;
        }
        else {
                s->size[r2] = s->size[r1] + s->size[r2];
                s->p[ r1 ] = r2;
        }
}

bool same_component(set_union *s, int s1, int s2)
{
        return ( find(s,s1) == find(s,s2) );
}
```

Analysis

On each union, the tree with fewer nodes becomes the child. But how tall can such a tree get as a function of the number of nodes in it? Consider the smallest possible tree of height h. Single-node trees have height 1. The smallest tree of height-2 has two nodes; from the union of two single-node trees. When do we increase the height? Merging in single-node trees won't do it, since they just become children of the rooted tree of height-2. Only when we merge two height-2 trees together do we get a tree of height-3, now with four nodes.

See the pattern? We must double the number of nodes in the tree to get an extra unit of height. How many doublings can we do before we use up all n nodes? At most, $\lg_2 n$ doublings can be performed. Thus, we can do both unions and finds in $O(\log n)$, good enough for Kruskal's algorithm. In fact, union-find can be done even faster, as discussed in Section 12.5 (page 385).

6.1.4 Variations on Minimum Spanning Trees

This minimum spanning tree algorithm has several interesting properties that help solve several closely related problems:

- *Maximum Spanning Trees* – Suppose an evil telephone company is contracted to connect a bunch of houses together; they will be paid a price proportional to the amount of wire they install. Naturally, they will build the most expensive spanning tree possible. The *maximum spanning tree* of any graph can be found by simply negating the weights of all edges and running Prim's algorithm. The most negative tree in the negated graph is the maximum spanning tree in the original.

  Most graph algorithms do not adapt so easily to negative numbers. Indeed, shortest path algorithms have trouble with negative numbers, and certainly do *not* generate the longest possible path using this technique.

- *Minimum Product Spanning Trees* – Suppose we seek the spanning tree that minimizes the product of edge weights, assuming all edge weights are positive. Since $\lg(a \cdot b) = \lg(a) + \lg(b)$, the minimum spanning tree on a graph whose edge weights are replaced with their logarithms gives the minimum product spanning tree on the original graph.

- *Minimum Bottleneck Spanning Tree* – Sometimes we seek a spanning tree that minimizes the maximum edge weight over all such trees. In fact, every minimum spanning tree has this property. The proof follows directly from the correctness of Kruskal's algorithm.

  Such bottleneck spanning trees have interesting applications when the edge weights are interpreted as costs, capacities, or strengths. A less efficient

but conceptually simpler way to solve such problems might be to delete all "heavy" edges from the graph and ask whether the result is still connected. These kind of tests can be done with simple BFS/DFS.

The minimum spanning tree of a graph is unique if all m edge weights in the graph are distinct. Otherwise the order in which Prim's/Kruskal's algorithm breaks ties determines which minimum spanning tree is returned.

There are two important variants of a minimum spanning tree that are *not* solvable with these techniques.

- *Steiner Tree* – Suppose we want to wire a bunch of houses together, but have the freedom to add extra intermediate vertices to serve as a shared junction. This problem is known as a *minimum Steiner tree*, and is discussed in the catalog in Section 16.10.

- *Low-degree Spanning Tree* – Alternately, what if we want to find the minimum spanning tree where the highest degree node in the tree is small? The lowest max-degree tree possible would be a simple path, and have $n - 2$ nodes of degree 2 with two endpoints of degree 1. A path that visits each vertex once is called a *Hamiltonian path*, and is discussed in the catalog in Section 16.5.

6.2 War Story: Nothing but Nets

I'd been tipped off about a small printed-circuit board testing company nearby in need of some algorithmic consulting. And so I found myself inside a nondescript building in a nondescript industrial park, talking with the president of Integri-Test and one of his lead technical people.

"We're leaders in robotic printed-circuit board testing devices. Our customers have very high reliability requirements for their PC-boards. They must check that each and every board has no wire breaks *before* filling it with components. This means testing that each and every pair of points on the board that are supposed to be connected *are* connected."

"How do you do the testing?" I asked.

"We have a robot with two arms, each with electric probes. The arms simultaneously contact both of the points to test whether two points are properly connected. If they are properly connected, then the probes will complete a circuit. For each net, we hold one arm fixed at one point and move the other to cover the rest of the points."

"Wait!" I cried. "What is a net?"

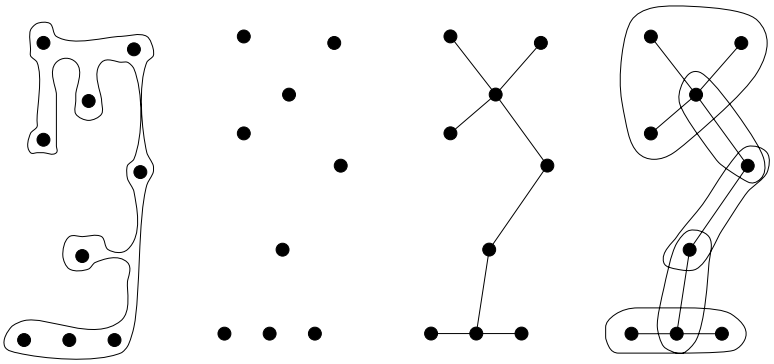

Figure 6.6: An example net showing (a) the metal connection layer, (b) the contact points, (c) their minimum spanning tree, and (d) the points partitioned into clusters

"Circuit boards are certain sets of points that are all connected together with a metal layer. This is what we mean by a net. Sometimes a net consists of two points—i.e. , an isolated wire. Sometimes a net can have 100 to 200 points, like all the connections to power or ground."

"I see. So you have a list of all the connections between pairs of points on the circuit board, and you want to trace out these wires."

He shook his head. "Not quite. The input for our testing program consists only of the net contact points, as shown in Figure 6.6(b). We don't know where the actual wires are, but we don't have to. All we must do is verify that all the points in a net are connected together. We do this by putting the left robot arm on the leftmost point in the net, and then have the right arm move around to all the other points in the net to test if they are all connected to the left point. So they must all be connected to each other."

I thought for a moment about what this meant. "OK. So your right arm has to visit all the other points in the net. How do you choose the order to visit them?"

The technical guy spoke up. "Well, we sort the points from left to right and then go in that order. Is that a good thing to do?"

"Have you ever heard of the traveling salesman problem?" I asked.

He was an electrical engineer, not a computer scientist. "No, what's that?"

"Traveling salesman is the name of the problem that you are trying to solve. Given a set of points to visit, how do you order them to minimize the travel time. Algorithms for the traveling salesman problem have been extensively studied. For small nets, you will be able to find the optimal tour by doing an exhaustive search. For big nets, there are heuristics that will get you very close to the optimal tour." I would have pointed them to Section 16.4 (page 533) if I had had this book handy.

The president scribbled down some notes and then frowned. "Fine. Maybe you can order the points in a net better for us. But that's not our real problem. When you watch our robot in action, the right arm sometimes has to run all the way to the right side of the board on a given net, while the left arm just sits there. It seems we would benefit by breaking nets into smaller pieces to balance things out."

I sat down and thought. The left and right arms each have interlocking TSP problems to solve. The left arm would move between the leftmost points of each net, while the right arm to visits all the other points in each net as ordered by the left TSP tour. By breaking each net into smaller nets we would avoid making the right arm cross all the way across the board. Further, a lot of little nets meant there would be more points in the left TSP, so each left-arm movement was likely to be short, too.

"You are right. We should win if we can break big nets into small nets. We want the nets to be small, both in the number of points and in physical area. But we must be sure that if we validate the connectivity of each small net, we will have confirmed that the big net is connected. One point in common between two little nets is sufficient to show that the bigger net formed by the two little nets is connected, since current can flow between any pair of points."

Now we had to break each net into overlapping pieces, where each piece was small. This is a clustering problem. Minimum spanning trees are often used for clustering, as discussed in Section 15.3 (page 484). In fact, that was the answer! We could find the minimum spanning tree of the net points and break it into little clusters whenever a spanning tree edge got too long. As shown in Figure 6.6(d), each cluster would share exactly one point in common with another cluster, with connectivity ensured because we are covering the edges of a spanning tree. The shape of the clusters will reflect the points in the net. If the points lay along a line across the board, the minimum spanning tree would be a path, and the clusters would be pairs of points. If the points all fell in a tight region, there would be one nice fat cluster for the right arm to scoot around.

So I explained the idea of constructing the minimum spanning tree of a graph. The boss listened, scribbled more notes, and frowned again.

"I like your clustering idea. But minimum spanning trees are defined on graphs. All you've got are points. Where do the weights of the edges come from?"

"Oh, we can think of it as a complete graph, where every pair of points are connected. The weight of the edge is defined as the distance between the two points. Or is it. . . ?"

I went back to thinking. The edge cost should reflect the travel time between between two points. While distance is related to travel time, it wasn't necessarily the same thing.

"Hey. I have a question about your robot. Does it take the same amount of time to move the arm left-right as it does up-down?"

They thought a minute. "Yeah, it does. We use the same type of motor to control horizontal and vertical movements. Since the two motors for each arm are

independent, we can simultaneously move each arm both horizontally and vertically."

"So the time to move both one foot left and one foot up is exactly the same as just moving one foot left? This means that the weight for each edge should *not* be the Euclidean distance between the two points, but the biggest difference between either the $x-$ or y-coordinate. This is something we call the L_∞ metric, but we can capture it by changing the edge weights in the graph. Anything else funny about your robots?" I asked.

"Well, it takes some time for the robot to come up to speed. We should probably also factor in acceleration and deceleration of the arms."

"Darn right. The more accurately you can model the time your arm takes to move between two points, the better our solution will be. But now we have a very clean formulation. Let's code it up and let's see how well it works!"

They were somewhat skeptical whether this approach would do any good, but agreed to think about it. A few weeks later they called me back and reported that the new algorithm reduced the distance traveled by about 30% over their previous approach, at a cost of a little more computational preprocessing. However, since their testing machine cost $200,000 a pop and a PC cost $2,000, this was an excellent tradeoff. It is particularly advantageous since the preprocessing need only be done once when testing multiple instances of a particular board design.

The key idea leading to the successful solution was modeling the job in terms of classical algorithmic graph problems. I smelled TSP the instant they started talking about minimizing robot motion. Once I realized that they were implicitly forming a star-shaped spanning tree to ensure connectivity, it was natural to ask whether the minimum spanning tree would perform any better. This idea led to clustering, and thus partitioning each net into smaller nets. Finally, by carefully designing our distance metric to accurately model the costs of the robot itself, we could incorporate such complicated properties (as acceleration) without changing our fundamental graph model or algorithm design.

> *Take-Home Lesson:* Most applications of graphs can be reduced to standard graph properties where well-known algorithms can be used. These include minimum spanning trees, shortest paths, and other problems presented in the catalog.

6.3 Shortest Paths

A *path* is a sequence of edges connecting two vertices. Since movie director Mel Brooks ("The Producers") is my father's sister's husband's cousin, there is a path in the friendship graph between me and him, shown in Figure 6.7—even though the two of us have never met. But if I were trying to impress how tight I am with Cousin Mel, I would be much better off saying that my Uncle Lenny grew up with him. I have a friendship path of length 2 to Cousin Mel through Uncle Lenny, while

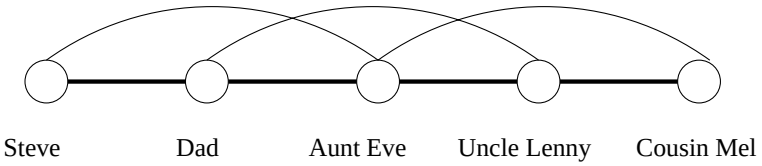

Figure 6.7: Mel Brooks is my father's sister's husband's cousin

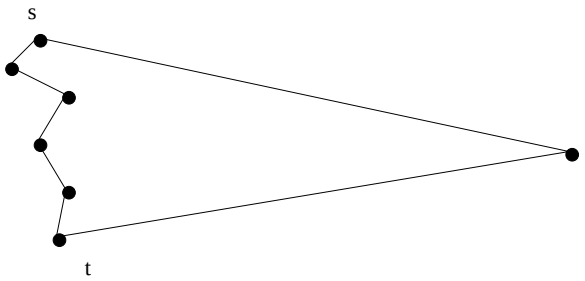

Figure 6.8: The shortest path from s to t may pass through many intermediate vertices

the path is of length 4 by blood and marriage. This multiplicity of paths hints at why finding the *shortest path* between two nodes is important and instructive, even in nontransportation applications.

The shortest path from s to t in an unweighted graph can be constructed using a breadth-first search from s. The minimum-link path is recorded in the breadth-first search tree, and it provides the shortest path when all edges have equal weight.

However, BFS does *not* suffice to find shortest paths in weighted graphs. The shortest weighted path might use a large number of edges, just as the shortest route (timewise) from home to office may involve complicated shortcuts using backroads, as shown in Figure 6.8.

In this section, we will present two distinct algorithms for finding the shortest paths in weighted graphs.

6.3.1 Dijkstra's Algorithm

Dijkstra's algorithm is the method of choice for finding shortest paths in an edge- and/or vertex-weighted graph. Given a particular start vertex s, it finds the shortest path from s to every other vertex in the graph, including your desired destination t.

Suppose the shortest path from s to t in graph G passes through a particular intermediate vertex x. Clearly, this path must contain the shortest path from s to x as its prefix, because if not, we could shorten our s-to-t path by using the shorter

s-to-x prefix. Thus, we must compute the shortest path from s to x before we find the path from s to t.

Dijkstra's algorithm proceeds in a series of rounds, where each round establishes the shortest path from s to *some* new vertex. Specifically, x is the vertex that minimizes $dist(s, v_i) + w(v_i, x)$ over all unfinished $1 \leq i \leq n$, where $w(i, j)$ is the length of the edge from i to j, and $dist(i, j)$ is the length of the shortest path between them.

This suggests a dynamic programming-like strategy. The shortest path from s to itself is trivial unless there are negative weight edges, so $dist(s, s) = 0$. If (s, y) is the lightest edge incident to s, then this implies that $dist(s, y) = w(s, y)$. Once we determine the shortest path to a node x, we check all the outgoing edges of x to see whether there is a better path from s to some unknown vertex through x.

```
ShortestPath-Dijkstra(G, s, t)
    known = {s}
    for i = 1 to n, dist[i] = ∞
    for each edge (s, v), dist[v] = w(s, v)
    last = s
    while (last ≠ t)
        select v_next, the unknown vertex minimizing dist[v]
        for each edge (v_next, x), dist[x] = min[dist[x], dist[v_next] + w(v_next, x)]
        last = v_next
        known = known ∪ {v_next}
```

The basic idea is very similar to Prim's algorithm. In each iteration, we add exactly one vertex to the tree of vertices for which we *know* the shortest path from s. As in Prim's, we keep track of the best path seen to date for all vertices outside the tree, and insert them in order of increasing cost.

The difference between Dijkstra's and Prim's algorithms is how they rate the desirability of each outside vertex. In the minimum spanning tree problem, all we cared about was the weight of the next potential tree edge. In shortest path, we want to include the closest outside vertex (in shortest-path distance) to s. This is a function of both the new edge weight *and* the distance from s to the tree vertex it is adjacent to.

Implementation

The pseudocode actually obscures how similar the two algorithms are. In fact, the change is very minor. Below, we give an implementation of Dijkstra's algorithm based on changing exactly three lines from our Prim's implementation—one of which is simply the name of the function!

```
dijkstra(graph *g, int start)      /* WAS prim(g,start) */
{
     int i;                    /* counter */
     edgenode *p;              /* temporary pointer */
     bool intree[MAXV+1];      /* is the vertex in the tree yet? */
     int distance[MAXV+1];     /* distance vertex is from start */
     int v;                    /* current vertex to process */
     int w;                    /* candidate next vertex */
     int weight;               /* edge weight */
     int dist;                 /* best current distance from start */

     for (i=1; i<=g->nvertices; i++) {
             intree[i] = FALSE;
             distance[i] = MAXINT;
             parent[i] = -1;
     }

     distance[start] = 0;
     v = start;

     while (intree[v] == FALSE) {
            intree[v] = TRUE;
            p = g->edges[v];
            while (p != NULL) {
                    w = p->y;
                    weight = p->weight;
/* CHANGED */              if (distance[w] > (distance[v]+weight)) {
/* CHANGED */                      distance[w] = distance[v]+weight;
/* CHANGED */                      parent[w] = v;
                       }
                       p = p->next;
               }

              v = 1;
              dist = MAXINT;
              for (i=1; i<=g->nvertices; i++)
                    if ((intree[i] == FALSE) && (dist > distance[i])) {
                           dist = distance[i];
                           v = i;
                       }
        }
}
```

This algorithm finds more than just the shortest path from s to t. It finds the shortest path from s to all other vertices. This defines a shortest path spanning tree rooted in s. For undirected graphs, this would be the breadth-first search tree, but in general it provides the shortest path from s to all other vertices.

Analysis

What is the running time of Dijkstra's algorithm? As implemented here, the complexity is $O(n^2)$. This is the same running time as a proper version of Prim's algorithm; except for the extension condition it *is* the same algorithm as Prim's.

The length of the shortest path from `start` to a given vertex t is exactly the value of `distance[t]`. How do we use `dijkstra` to find the actual path? We follow the backward `parent` pointers from t until we hit `start` (or `-1` if no such path exists), exactly as was done in the `find_path()` routine of Section 5.6.2 (page 165).

Dijkstra works correctly only on graphs without negative-cost edges. The reason is that midway through the execution we may encounter an edge with weight so negative that it changes the cheapest way to get from s to some other vertex already in the tree. Indeed, the most cost-effective way to get from your house to your next-door neighbor would be repeatedly through the lobby of any bank offering you enough money to make the detour worthwhile.

Most applications do not feature negative-weight edges, making this discussion academic. Floyd's algorithm, discussed below, works correctly unless there are negative cost cycles, which grossly distort the shortest-path structure. Unless that bank limits its reward to one per customer, you might so benefit by making an infinite number of trips through the lobby that you would *never* decide to actually reach your destination!

Stop and Think: Shortest Path with Node Costs

Problem: Suppose we are given a graph whose weights are on the vertices, instead of the edges. Thus, the cost of a path from x to y is the sum of the weights of all vertices on the path.

Give an efficient algorithm for finding shortest paths on vertex-weighted graphs.

Solution: A natural idea would be to adapt the algorithm we have for edge-weighted graphs (Dijkstra's) to the new vertex-weighted domain. It should be clear that we can do it. We replace any reference to the weight of an edge with the weight of the destination vertex. This can be looked up as needed from an array of vertex weights.

However, my preferred approach would leave Dijkstra's algorithm intact and instead concentrate on constructing an edge-weighted graph on which Dijkstra's

algorithm will give the desired answer. Set the weight of each directed edge (i, j) in the input graph to the cost of vertex j. Dijkstra's algorithm now does the job.

This technique can be extended to a variety of different domains, such as when there are costs on both vertices and edges. ∎

6.3.2 All-Pairs Shortest Path

Suppose you want to find the "center" vertex in a graph—the one that minimizes the longest or average distance to all the other nodes. This might be the best place to start a new business. Or perhaps you need to know a graph's *diameter*—the longest shortest-path distance over all pairs of vertices. This might correspond to the longest possible time it takes a letter or network packet to be delivered. These and other applications require computing the shortest path between all pairs of vertices in a given graph.

We could solve *all-pairs shortest path* by calling Dijkstra's algorithm from each of the n possible starting vertices. But Floyd's all-pairs shortest-path algorithm is a slick way to construct this $n \times n$ distance matrix from the original weight matrix of the graph.

Floyd's algorithm is best employed on an adjacency matrix data structure, which is no extravagance since we must store all n^2 pairwise distances anyway. Our `adjacency_matrix` type allocates space for the largest possible matrix, and keeps track of how many vertices are in the graph:

```
typedef struct {
     int weight[MAXV+1][MAXV+1];  /* adjacency/weight info */
     int nvertices;               /* number of vertices in graph */
} adjacency_matrix;
```

The critical issue in an adjacency matrix implementation is how we denote the edges absent from the graph. A common convention for unweighted graphs denotes graph edges by 1 and non-edges by 0. This gives exactly the wrong interpretation if the numbers denote edge weights, for the non-edges get interpreted as a free ride between vertices. Instead, we should initialize each non-edge to `MAXINT`. This way we can both test whether it is present and automatically ignore it in shortest-path computations, since only real edges will be used, provided `MAXINT` is less than the diameter of your graph.

There are several ways to characterize the shortest path between two nodes in a graph. The Floyd-Warshall algorithm starts by numbering the vertices of the graph from 1 to n. We use these numbers not to label the vertices, but to order them. Define $W[i, j]^k$ to be the length of the shortest path from i to j using only vertices numbered from $1, 2, ..., k$ as possible intermediate vertices.

What does this mean? When $k = 0$, we are allowed no intermediate vertices, so the only allowed paths are the original edges in the graph. Thus the initial

all-pairs shortest-path matrix consists of the initial adjacency matrix. We will perform n iterations, where the kth iteration allows only the first k vertices as possible intermediate steps on the path between each pair of vertices x and y.

At each iteration, we allow a richer set of possible shortest paths by adding a new vertex as a possible intermediary. Allowing the kth vertex as a stop helps only if there is a short path that goes through k, so

$$W[i,j]^k = \min(W[i,j]^{k-1}, W[i,k]^{k-1} + W[k,j]^{k-1})$$

The correctness of this is somewhat subtle, and I encourage you to convince yourself of it. But there is nothing subtle about how simple the implementation is:

```
floyd(adjacency_matrix *g)
{
    int i,j;                    /* dimension counters */
    int k;                      /* intermediate vertex counter */
    int through_k;              /* distance through vertex k */

    for (k=1; k<=g->nvertices; k++)
            for (i=1; i<=g->nvertices; i++)
                 for (j=1; j<=g->nvertices; j++) {
                       through_k = g->weight[i][k]+g->weight[k][j];
                       if (through_k < g->weight[i][j])
                               g->weight[i][j] = through_k;
                 }
}
```

The Floyd-Warshall all-pairs shortest path runs in $O(n^3)$ time, which is asymptotically no better than n calls to Dijkstra's algorithm. However, the loops are so tight and the program so short that it runs better in practice. It is notable as one of the rare graph algorithms that work better on adjacency matrices than adjacency lists.

The output of Floyd's algorithm, as it is written, does not enable one to reconstruct the actual shortest path between any given pair of vertices. These paths can be recovered if we retain a parent matrix P of our choice of the last intermediate vertex used for each vertex pair (x, y). Say this value is k. The shortest path from x to y is the concatenation of the shortest path from x to k with the shortest path from k to y, which can be reconstructed recursively given the matrix P. Note, however, that most all-pairs applications need only the resulting distance matrix. These jobs are what Floyd's algorithm was designed for.

6.3.3 Transitive Closure

Floyd's algorithm has another important application, that of computing *transitive closure*. In analyzing a directed graph, we are often interested in which vertices are reachable from a given node.

As an example, consider the *blackmail graph*, where there is a directed edge (i, j) if person i has sensitive-enough private information on person j so that i can get j to do whatever he wants. You wish to hire one of these n people to be your personal representative. Who has the most power in terms of blackmail potential?

A simplistic answer would be the vertex of highest degree, but an even better representative would be the person who has blackmail chains leading to the most other parties. Steve might only be able to blackmail Miguel directly, but if Miguel can blackmail everyone else then Steve is the man you want to hire.

The vertices reachable from any single node can be computed using breadth-first or depth-first searches. But the whole batch can be computed using an all-pairs shortest-path. If the shortest path from i to j remains `MAXINT` after running Floyd's algorithm, you can be sure no directed path exists from i to j. Any vertex pair of weight less than `MAXINT` must be reachable, both in the graph-theoretic and blackmail senses of the word.

Transitive closure is discussed in more detail in the catalog in Section 15.5.

6.4 War Story: Dialing for Documents

I was part of a group visiting Periphonics, which was then an industry leader in building telephone voice-response systems. These are more advanced versions of the *Press 1 for more options, Press 2 if you didn't press 1* telephone systems that blight everyone's lives. We were being given the standard tour when someone from our group asked, "Why don't you guys use voice recognition for data entry. It would be a lot less annoying than typing things out on the keypad."

The tour guide reacted smoothly. "Our customers have the option of incorporating speech recognition into our products, but very few of them do. User-independent, connected-speech recognition is not accurate enough for most applications. Our customers prefer building systems around typing text on the telephone keyboards."

"Prefer typing, my pupik!" came a voice from the rear of our group. "I *hate* typing on a telephone. Whenever I call my brokerage house to get stock quotes some machine tells me to type in the three letter code. To make things worse, I have to hit two buttons to type in one letter, in order to distinguish between the three letters printed on each key of the telephone. I hit the 2 key and it says Press 1 for A, Press 2 for B, Press 3 for C. Pain in the neck if you ask me."

"Maybe you don't have to hit two keys for each letter!" I chimed in. "Maybe the system could figure out the correct letter from context!"

"There isn't a whole lot of context when you type in three letters of stock market code."

"Sure, but there would be plenty of context if we typed in English sentences. I'll bet that we could reconstruct English text correctly if they were typed in a telephone at one keystroke per letter."

The guy from Periphonics gave me a disinterested look, then continued the tour. But when I got back to the office, I decided to give it a try.

Not all letters are equally likely to be typed on a telephone. In fact, not all letters *can* be typed, since Q and Z are not labeled on a standard American telephone. Therefore, we adopted the convention that Q, Z, and "space" all sat on the * key. We could take advantage of the uneven distribution of letter frequencies to help us decode the text. For example, if you hit the 3 key while typing English, you more likely meant to type an E than either a D or F. By taking into account the frequencies of a window of three characters (trigrams), we could predict the typed text. This is what happened when I tried it on the Gettysburg Address:

> enurraore ane reten yeasr ain our ectherr arotght eosti on ugis aootinent a oey oation aoncdivee in licesty ane eedicatee un uhe rrorosition uiat all oen are arectee e ual
>
> ony ye are enichde in a irect aitil yar uestini yhethes uiat oatioo or aoy oation ro aoncdivee ane ro eedicatee aan loni eneure ye are oet on a irect aattlediele oe uiat yar ye iate aone un eedicate a rostion oe uiat eiele ar a einal restini rlace eor uiore yin iere iate uhdis lives uiat uhe oation ogght live it is aluniethes eittini ane rrores uiat ye rioule en ugir
>
> att in a laries reore ye aan oou eedicate ye aan oou aoorearate ye aan oou ialloy ugis iroune the arate oen litini ane eeae yin rustgilee iere iate aoorearatee it ear aante our roor rowes un ade or eeuraat the yople yill little oote oor loni renences yiat ye ray iere att it aan oetes eosiet yiat uhfy eie iere it is eor ur uhe litini rathes un ae eedicatee iere un uhe undiniside yopl yhici uhfy yin entght iere iate uiur ear ro onaky aetancde it is rathes eor ur un ae iere eedicatee un uhe irect uarl rencinini adeore ur uiat eron uhere ioooree eeae ye uale inarearee eeuotion uo tiat aaure eor yhici uhfy iere iate uhe lart eull oearure oe eeuotioo tiat ye iere iggily rerolue uiat uhere eeae riall oou iate eide io

The trigram statistics did a decent job of translating it into Greek, but a terrible job of transcribing English. One reason was clear. This algorithm knew nothing about English words. If we coupled it with a dictionary, we might be onto something. But two words in the dictionary are often represented by the exact same string of phone codes. For an extreme example, the code string "22737" collides with eleven distinct English words, including *cases, cares, cards, capes, caper*, and *bases*. For our next attempt, we reported the unambiguous characters of any words that collided in the dictionary, and used trigrams to fill in the rest of the characters. We were rewarded with:

> eourscore and seven yearr ain our eatherr brought forth on this continent azoey nation conceivee in liberty and dedicatee uo uhe proposition that all men are createe equal
>
> ony ye are engagee in azipeat civil yar uestioi whether that nation or aoy nation ro conceivee and ro dedicatee aan long endure ye are oet on azipeat battlefield oe that yar ye iate aone uo dedicate a rostion oe that field ar a final perthni place for those yin here iate their lives that uhe nation oight live it is altogether fittinizane proper that ye should en this
>
> aut in a larges sense ye aan oou dedicate ye aan oou consecrate ye aan oou hallow this ground the arate men litioi and deae yin strugglee here iate consecratee it ear above our roor power uo ade or detract the world will little oote oor long remember what ye

ray here aut it aan meter forget what uhfy die here it is for ur uhe litioi rather uo ae dedicatee here uo uhe toeioisgee york which uhfy yin fought here iate thus ear ro mocky advancee it is rather for ur uo ae here dedicatee uo uhe great task renagogoi adfore ur that from there honoree deae ye uale increasee devotion uo that aause for which uhfy here iate uhe last eull measure oe devotion that ye here highky resolve that there deae shall oou iate fide io vain that this nation under ioe shall iate azoey birth oe freedom and that ioternmenu oe uhe people ay uhe people for uhe people shall oou perish from uhe earth

If you were a student of American history, maybe you could recognize it, but you certainly couldn't read it. Somehow, we had to distinguish between the different dictionary words that got hashed to the same code. We could factor in the relative popularity of each word, but this still made too many mistakes.

At this point, I started working with Harald Rau on the project, who proved to be a great collaborator. First, he was a bright and persistent graduate student. Second, as a native German speaker, he believed every lie I told him about English grammar.

Harald built up a phone code reconstruction program along the lines of Figure 6.9. It worked on the input one sentence at a time, identifying dictionary words that matched each code string. The key problem was how to incorporate grammatical constraints.

"We can get good word-use frequencies and grammatical information from a big text database called the Brown Corpus. It contains thousands of typical English sentences, each parsed according to parts of speech. But how do we factor it all in?" Harald asked.

"Let's think about it as a graph problem," I suggested.

"*Graph problem?* What graph problem? Where is there even a graph?"

"Think of a sentence as a series of phone tokens, each representing a word in the sentence. Each phone token has a list of words from the dictionary that match it. How can we choose which one is right? Each possible sentence interpretation can be thought of as a path in a graph. The vertices of this graph are the complete set of possible word choices. There will be an edge from each possible choice for the ith word to each possible choice for the $(i+1)$st word. The cheapest path across this graph defines the best interpretation of the sentence."

"But all the paths look the same. They have the same number of edges. Wait. Now I see! We have to add weight to the edges to make the paths different."

"Exactly! The cost of an edge will reflect how likely it is that we will travel through the given pair of words. Perhaps we can count how often that pair of words occurred together in previous texts. Or we can weigh them by the part of speech of each word. Maybe nouns don't like to be next to nouns as much as they like being next to verbs."

"It will be hard to keep track of word-pair statistics, since there are so many of them. But we certainly know the frequency of each word. How can we factor that into things?"

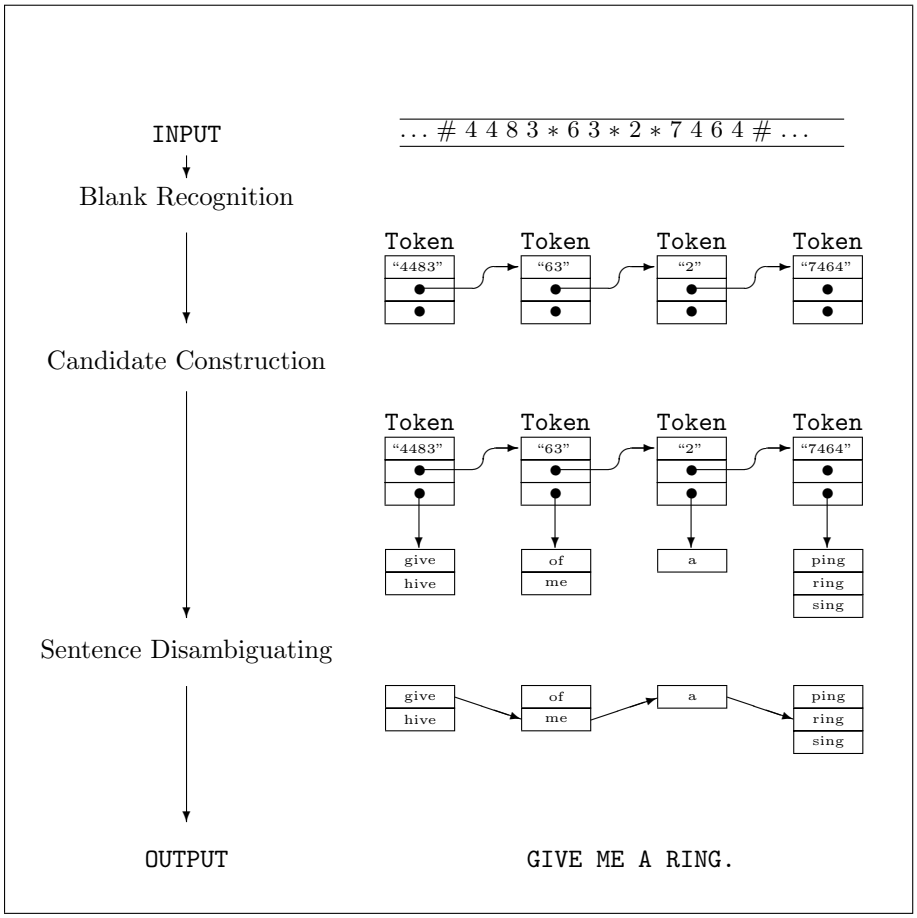

Figure 6.9: The phases of the telephone code reconstruction process

"We can pay a cost for walking through a particular vertex that depends upon the frequency of the word. Our best sentence will be given by the shortest path across the graph."

"But how do we figure out the relative weights of these factors?"

"First try what seems natural to you and then we can experiment with it."

Harald incorporated this shortest-path algorithm. With proper grammatical and statistical constraints, the system performed great. Look at the Gettysburg Address now, with all the reconstruction errors highlighted:

FOURSCORE AND SEVEN YEARS AGO OUR FATHERS BROUGHT FORTH ON THIS CONTINENT A NEW NATION CONCEIVED IN LIBERTY AND DEDICATED TO THE PROPOSITION THAT ALL MEN ARE CREATED EQUAL. NOW WE ARE

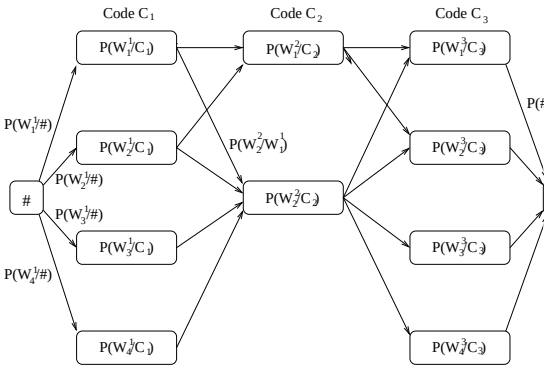

Figure 6.10: The minimum-cost path defines the best interpretation for a sentence

Text	characters	characters correct	non-blanks correct	words correct	time per character
Clinton Speeches	1,073,593	99.04%	98.86%	97.67%	0.97ms
Herland	278,670	98.24%	97.89%	97.02%	0.97ms
Moby Dick	1,123,581	96.85%	96.25%	94.75%	1.14ms
Bible	3,961,684	96.20%	95.39%	95.39%	1.33ms
Shakespeare	4,558,202	95.20%	94.21%	92.86%	0.99ms

Figure 6.11: Telephone-code reconstruction applied to several text samples

ENGAGED IN A GREAT CIVIL WAR TESTING WHETHER THAT NATION OR ANY NATION SO CONCEIVED AND SO DEDICATED CAN LONG ENDURE. WE ARE MET ON A GREAT BATTLEFIELD OF THAT **WAS**. WE HAVE COME TO DEDICATE A PORTION OF THAT FIELD AS A FINAL **SERVING** PLACE FOR THOSE WHO HERE **HAVE** THEIR LIVES THAT THE NATION MIGHT LIVE. IT IS ALTOGETHER FITTING AND PROPER THAT WE SHOULD DO THIS. BUT IN A LARGER SENSE WE CAN NOT DEDICATE WE CAN NOT CONSECRATE WE CAN NOT HALLOW THIS GROUND. THE BRAVE MEN LIVING AND DEAD WHO STRUGGLED HERE HAVE CONSECRATED IT FAR ABOVE OUR POOR POWER TO ADD OR DETRACT. THE WORLD WILL LITTLE NOTE NOR LONG REMEMBER WHAT WE SAY HERE BUT IT CAN NEVER FORGET WHAT THEY DID HERE. IT IS FOR US THE LIVING RATHER TO BE DEDICATED HERE TO THE UNFINISHED WORK WHICH THEY WHO FOUGHT HERE HAVE THUS FAR SO NOBLY ADVANCED. IT IS RATHER FOR US TO BE HERE DEDICATED TO THE GREAT TASK REMAINING BEFORE US THAT FROM THESE HONORED DEAD WE TAKE INCREASED DEVOTION TO THAT CAUSE FOR WHICH THEY HERE **HAVE** THE LAST FULL MEASURE OF DEVOTION THAT WE HERE HIGHLY RESOLVE THAT THESE DEAD SHALL NOT HAVE DIED IN VAIN THAT THIS NATION UNDER GOD SHALL HAVE A NEW BIRTH OF FREEDOM AND THAT GOVERNMENT OF THE PEOPLE BY THE PEOPLE FOR THE PEOPLE SHALL NOT PERISH FROM THE EARTH.

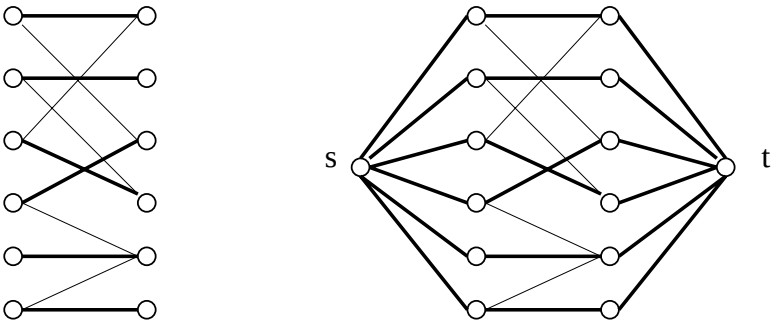

Figure 6.12: Bipartite graph with a maximum matching highlighted (on left). The corresponding network flow instance highlighting the maximum $s-t$ flow (on right).

While we still made a few mistakes, the results are clearly good enough for many applications. Periphonics certainly thought so, for they licensed our program to incorporate into their products. Figure 6.11 shows that we were able to reconstruct correctly over 99% of the characters in a megabyte of President Clinton's speeches, so if Bill had phoned them in, we would certainly be able to understand what he was saying. The reconstruction time is fast enough, indeed faster than you can type it in on the phone keypad.

The constraints for many pattern recognition problems can be naturally formulated as shortest path problems in graphs. In fact, there is a particularly convenient dynamic programming solution for these problems (the Viterbi algorithm) that is widely used in speech and handwriting recognition systems. Despite the fancy name, the Viterbi algorithm is basically solving a shortest path problem on a DAG. Hunting for a graph formulation to solve any given problem is often a good idea.

6.5 Network Flows and Bipartite Matching

Edge-weighted graphs can be interpreted as a network of pipes, where the weight of edge (i, j) determines the *capacity* of the pipe. Capacities can be thought of as a function of the cross-sectional area of the pipe. A wide pipe might be able to carry 10 units of flow in a given time, where as a narrower pipe might only carry 5 units. The *network flow problem* asks for the maximum amount of flow which can be sent from vertices s to t in a given weighted graph G while respecting the maximum capacities of each pipe.

6.5.1 Bipartite Matching

While the network flow problem is of independent interest, its primary importance is in to solving other important graph problems. A classic example is bipartite matching. A *matching* in a graph $G = (V, E)$ is a subset of edges $E' \subset E$ such that no two edges of E' share a vertex. A matching pairs off certain vertices such that every vertex is in, at most, one such pair, as shown in Figure 6.12.

Graph G is *bipartite* or *two-colorable* if the vertices can be divided into two sets, L and R, such that all edges in G have one vertex in L and one vertex in R. Many naturally defined graphs are bipartite. For example, certain vertices may represent jobs to be done and the remaining vertices represent people who can potentially do them. The existence of edge (j, p) means that job j can be done by person p. Or let certain vertices represent boys and certain vertices represent girls, with edges representing compatible pairs. Matchings in these graphs have natural interpretations as job assignments or as marriages, and are the focus of Section 15.6 (page 498).

The largest bipartite matching can be readily found using network flow. Create a *source* node s that is connected to every vertex in L by an edge of weight 1. Create a *sink* node t and connect it to every vertex in R by an edge of weight 1. Finally, assign each edge in the bipartite graph G a weight of 1. Now, the maximum possible flow from s to t defines the largest matching in G. Certainly we can find a flow as large as the matching by using only the matching edges and their source-to-sink connections. Further, there can be no greater possible flow. How can we ever hope to get more than one flow unit through any vertex?

6.5.2 Computing Network Flows

Traditional network flow algorithms are based on the idea of *augmenting paths*, and repeatedly finding a path of positive capacity from s to t and adding it to the flow. It can be shown that the flow through a network is optimal if and only if it contains no augmenting path. Since each augmentation adds to the flow, we must eventually find the global maximum.

The key structure is the *residual flow graph*, denoted as $R(G, f)$, where G is the input graph and f is the current flow through G. This directed, edge-weighted $R(G, f)$ contains the same vertices as G. For each edge (i, j) in G with capacity $c(i, j)$ and flow $f(i, j)$, $R(G, f)$ may contain two edges:

(i) an edge (i, j) with weight $c(i, j) - f(i, j)$, if $c(i, j) - f(i, j) > 0$ and

(ii) an edge (j, i) with weight $f(i, j)$, if $f(i, j) > 0$.

The presence of edge (i, j) in the residual graph indicates that positive flow can be pushed from i to j. The weight of the edge gives the exact amount that can be pushed. A path in the residual flow graph from s to t implies that more flow can be pushed from s to t and the minimum edge weight on this path defines the amount of extra flow that can be pushed.

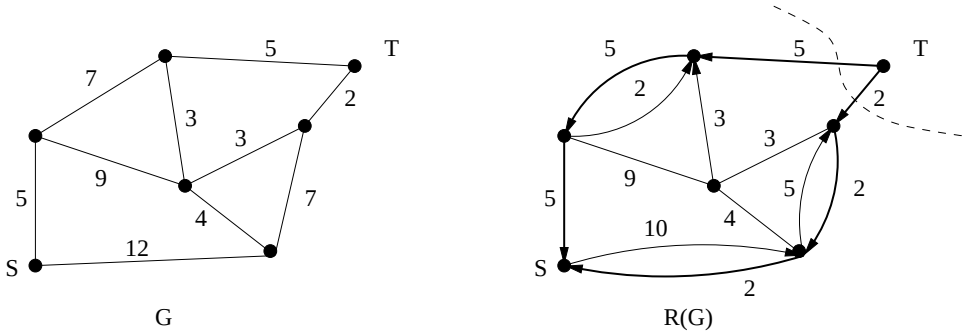

Figure 6.13: Maximum $s-t$ flow in a graph G (on left) showing the associated residual graph $R(G)$ and minimum $s-t$ cut (dotted line near t)

Figure 6.13 illustrates this idea. The maximum $s-t$ flow in graph G is 7. Such a flow is revealed by the two directed t to s paths in the residual graph $R(G)$ of capacities $2+5$, respectively. These flows completely saturate the capacity of the two edges incident to vertex t, so no augmenting path remains. Thus the flow is optimal. A set of edges whose deletion separates s from t (like the two edges incident to t) is called an s-t cut. Clearly, no s to t flow can exceed the weight of the minimum such cut. In fact, a flow equal to the minimum cut is always possible.

Take-Home Lesson: The maximum flow from s to t always equals the weight of the minimum s-t cut. Thus, flow algorithms can be used to solve general edge and vertex connectivity problems in graphs.

Implementation

We cannot do full justice to the theory of network flows here. However, it is instructive to see how augmenting paths can be identified and the optimal flow computed.

For each edge in the residual flow graph, we must keep track of both the amount of flow currently going through the edge, as well as its remaining *residual* capacity. Thus, we must modify our `edge` structure to accommodate the extra fields:

```
typedef struct {
        int v;                      /* neighboring vertex */
        int capacity;               /* capacity of edge */
        int flow;                   /* flow through edge */
        int residual;               /* residual capacity of edge */
        struct edgenode *next;      /* next edge in list */
} edgenode;
```

We use a breadth-first search to look for any path from source to sink that increases the total flow, and use it to augment the total. We terminate with the optimal flow when no such *augmenting* path exists.

```
netflow(flow_graph *g, int source, int sink)
{
      int volume;          /* weight of the augmenting path */

      add_residual_edges(g);

      initialize_search(g);
      bfs(g,source);

      volume = path_volume(g, source, sink, parent);

      while (volume > 0) {
              augment_path(g,source,sink,parent,volume);
              initialize_search(g);
              bfs(g,source);
              volume = path_volume(g, source, sink, parent);
      }
}
```

Any augmenting path from source to sink increases the flow, so we can use `bfs` to find such a path in the appropriate graph. We only consider network edges that have remaining capacity or, in other words, positive residual flow. The predicate below helps `bfs` distinguish between saturated and unsaturated edges:

```
bool valid_edge(edgenode *e)
{
        if (e->residual > 0) return (TRUE);
        else return(FALSE);
}
```

Augmenting a path transfers the maximum possible volume from the residual capacity into positive flow. This amount is limited by the path-edge with the smallest amount of residual capacity, just as the rate at which traffic can flow is limited by the most congested point.

```
int path_volume(flow_graph *g, int start, int end, int parents[])
{
     edgenode *e;                    /* edge in question */
     edgenode *find_edge();

     if (parents[end] == -1) return(0);

     e = find_edge(g,parents[end],end);

     if (start == parents[end])
             return(e->residual);
     else
             return( min(path_volume(g,start,parents[end],parents),
                         e->residual) );
}


edgenode *find_edge(flow_graph *g, int x, int y)
{
        edgenode *p;                    /* temporary pointer */

        p = g->edges[x];

        while (p != NULL) {
                if (p->v == y) return(p);
                p = p->next;
        }

        return(NULL);
}
```

Sending an additional unit of flow along directed edge (i, j) reduces the residual capacity of edge (i, j) but *increases* the residual capacity of edge (j, i). Thus, the act of augmenting a path requires modifying both forward and reverse edges for each link on the path.

```
augment_path(flow_graph *g, int start, int end, int parents[], int volume)
{
        edgenode *e;                    /* edge in question */
        edgenode *find_edge();

        if (start == end) return;

        e = find_edge(g,parents[end],end);
        e->flow += volume;
        e->residual -= volume;

        e = find_edge(g,end,parents[end]);
        e->residual += volume;

        augment_path(g,start,parents[end],parents,volume);
}
```

Initializing the flow graph requires creating directed flow edges (i, j) and (j, i) for each network edge $e = (i, j)$. Initial flows are all set to 0. The initial residual flow of (i, j) is set to the capacity of e, while the initial residual flow of (j, i) is set to 0.

Analysis

The augmenting path algorithm above eventually converges on the the optimal solution. However, each augmenting path may add only a little to the total flow, so, in principle, the algorithm might take an arbitrarily long time to converge.

However, Edmonds and Karp [EK72] proved that always selecting a *shortest* unweighted augmenting path guarantees that $O(n^3)$ augmentations suffice for optimization. In fact, the Edmonds-Karp algorithm is what is implemented above, since a breadth-first search from the source is used to find the next augmenting path.

6.6 Design Graphs, Not Algorithms

Proper modeling is the key to making effective use of graph algorithms. We have defined several graph properties, and developed algorithms for computing them. All told, about two dozen different graph problems are presented in the catalog, mostly in Sections 15 and 16. These classical graph problems provide a framework for modeling most applications.

The secret is learning to design graphs, not algorithms. We have already seen a few instances of this idea:

- The *maximum* spanning tree can be found by negating the edge weights of the input graph G and using a *minimum* spanning tree algorithm on the result. The most negative weight spanning tree will define the maximum weight tree in G.

- To solve bipartite matching, we constructed a special network flow graph such that the maximum flow corresponds to a maximum cardinality matching.

The applications below demonstrate the power of proper modeling. Each arose in a real-world application, and each can be modeled as a graph problem. Some of the modelings are quite clever, but they illustrate the versatility of graphs in representing relationships. As you read a problem, try to devise an appropriate graph representation before peeking to see how we did it.

Stop and Think: The Pink Panther's Passport to Peril

Problem: "I'm looking for an algorithm to design natural routes for video-game characters to follow through an obstacle-filled room. How should I do it?"

Solution: Presumably the desired route should look like a path that an intelligent being would choose. Since intelligent beings are either lazy or efficient, this should be modeled as a shortest path problem.

But what is the graph? One approach might be to lay a grid of points in the room. Create a vertex for each grid point that is a valid place for the character to stand; i.e. , that does not lie within an obstacle. There will be an edge between any pair of nearby vertices, weighted proportionally to the distance between them. Although direct geometric methods are known for shortest paths (see Section 15.4 (page 489)), it is easier to model this discretely as a graph. ∎

Stop and Think: Ordering the Sequence

Problem: "A DNA sequencing project generates experimental data consisting of small fragments. For each given fragment f, we know certain other fragments are forced to lie to the left of f, and certain other fragments are forced to be to the right of f. How can we find a consistent ordering of the fragments from left to right that satisfies all the constraints?"

Solution: Create a directed graph, where each fragment is assigned a unique vertex. Insert a directed edge $(\overrightarrow{l, f})$ from any fragment l that is forced to be to the left

of f, and a directed edge $(\overrightarrow{f, r})$ to any fragment r forced to be to the right of f. We seek an ordering of the vertices such that all the edges go from left to right. This is a *topological sort* of the resulting directed acyclic graph. The graph must be acyclic, because cycles make finding a consistent ordering impossible. ∎

Stop and Think: Bucketing Rectangles

Problem: "In my graphics work I need to solve the following problem. Given an arbitrary set of rectangles in the plane, how can I distribute them into a minimum number of buckets such that no subset of rectangles in any given bucket intersects another? In other words, there can not be any overlapping area between two rectangles in the same bucket."

Solution: We formulate a graph where each vertex is a rectangle, and there is an edge if two rectangles intersect. Each bucket corresponds to an *independent set* of rectangles, so there is no overlap between any two. A *vertex coloring* of a graph is a partition of the vertices into independent sets, so minimizing the number of colors is exactly what you want. ∎

Stop and Think: Names in Collision

Problem: "In porting code from UNIX to DOS, I have to shorten several hundred file names down to at most 8 characters each. I can't just use the first eight characters from each name, because "filename1" and "filename2" would be assigned the exact same name. How can I meaningfully shorten the names while ensuring that they do not collide?"

Solution: Construct a bipartite graph with vertices corresponding to each original file name f_i for $1 \leq i \leq n$, as well as a collection of acceptable shortenings for each name $f_{i1}, \ldots, f_{ik}$. Add an edge between each original and shortened name. We now seek a set of n edges that have no vertices in common, so each file name is mapped to a distinct acceptable substitute. *Bipartite matching*, discussed in Section 15.6 (page 498), is exactly this problem of finding an independent set of edges in a graph. ∎

Stop and Think: Separate the Text

Problem: "We need a way to separate the lines of text in the optical character-recognition system that we are building. Although there is some white space between the lines, problems like noise and the tilt of the page makes it hard to find. How can we do line segmentation?

Solution: Consider the following graph formulation. Treat each pixel in the image as a vertex in the graph, with an edge between two neighboring pixels. The weight of this edge should be proportional to how dark the pixels are. A segmentation between two lines is a path in this graph from the left to right side of the page. We seek a relatively straight path that avoids as much blackness as possible. This suggests that the *shortest path* in the pixel graph will likely find a good line segmentation. ∎

Take-Home Lesson: Designing novel graph algorithms is very hard, so don't do it. Instead, try to design graphs that enable you to use classical algorithms to model your problem.

Chapter Notes

Network flows are an advanced algorithmic technique, and recognizing whether a particular problem can be solved by network flow requires experience. We point the reader to books by Cook and Cunningham [CC97] and Ahuja, Magnanti, and Orlin [AMO93] for more detailed treatments of the subject.

The augmenting path method for network flows is due to Ford and Fulkerson [FF62]. Edmonds and Karp [EK72] proved that always selecting a *shortest* geodesic augmenting path guarantees that $O(n^3)$ augmentations suffice for optimization.

The phone code reconstruction system that was the subject of the war story is described in more technical detail in [RS96].

6.7 Exercises

Simulating Graph Algorithms

6-1. *[3]* For the graphs in Problem 5-1:

(a) Draw the spanning forest after every iteration of the main loop in Kruskal's algorithm.

(b) Draw the spanning forest after every iteration of the main loop in Prim's algorithm.

(c) Find the shortest path spanning tree rooted in A.

(d) Compute the maximum flow from A to H.

Minimum Spanning Trees

6-2. *[3]* Is the path between two vertices in a minimum spanning tree necessarily a shortest path between the two vertices in the full graph? Give a proof or a counterexample.

6-3. *[3]* Assume that all edges in the graph have distinct edge weights (i.e. , no pair of edges have the same weight). Is the path between a pair of vertices in a minimum spanning tree necessarily a shortest path between the two vertices in the full graph? Give a proof or a counterexample.

6-4. *[3]* Can Prim's and Kruskal's algorithm yield different minimum spanning trees? Explain why or why not.

6-5. *[3]* Does either Prim's and Kruskal's algorithm work if there are negative edge weights? Explain why or why not.

6-6. *[5]* Suppose we are *given* the minimum spanning tree T of a given graph G (with n vertices and m edges) and a new edge $e = (u, v)$ of weight w that we will add to G. Give an efficient algorithm to find the minimum spanning tree of the graph $G + e$. Your algorithm should run in $O(n)$ time to receive full credit.

6-7. *[5]* (a) Let T be a minimum spanning tree of a weighted graph G. Construct a new graph G' by adding a weight of k to every edge of G. Do the edges of T form a minimum spanning tree of G'? Prove the statement or give a counterexample.

(b) Let $P = \{s, \ldots, t\}$ describe a shortest weighted path between vertices s and t of a weighted graph G. Construct a new graph G' by adding a weight of k to every edge of G. Does P describe a shortest path from s to t in G'? Prove the statement or give a counterexample.

6-8. *[5]* Devise and analyze an algorithm that takes a weighted graph G and finds the smallest change in the cost to a non-MST edge that would cause a change in the minimum spanning tree of G. Your algorithm must be correct and run in polynomial time.

6-9. *[4]* Consider the problem of finding a minimum weight connected subset T of edges from a weighted connected graph G. The weight of T is the sum of all the edge weights in T.

(a) Why is this problem not just the minimum spanning tree problem? Hint: think negative weight edges.

(b) Give an efficient algorithm to compute the minimum weight connected subset T.

6-10. *[4]* Let $G = (V, E)$ be an undirected graph. A set $F \subseteq E$ of edges is called a *feedback-edge set* if every cycle of G has at least one edge in F.

(a) Suppose that G is unweighted. Design an efficient algorithm to find a minimum-size feedback-edge set.

(b) Suppose that G is a weighted undirected graph with positive edge weights. Design an efficient algorithm to find a minimum-weight feedback-edge set.

6-11. *[5]* Modify Prim's algorithm so that it runs in time $O(n \log k)$ on a graph that has only k different edges costs.

Union-Find

6-12. *[5]* Devise an efficient data structure to handle the following operations on a weighted directed graph:

(a) Merge two given components.

(b) Locate which component contains a given vertex v.

(c) Retrieve a minimum edge from a given component.

6-13. *[5]* Design a data structure that can perform a sequence of, m *union* and *find* operations on a universal set of n elements, consisting of a sequence of all *unions* followed by a sequence of all *finds*, in time $O(m + n)$.

Shortest Paths

6-14. *[3]* The *single-destination shortest path* problem for a directed graph seeks the shortest path *from* every vertex to a specified vertex v. Give an efficient algorithm to solve the single-destination shortest paths problem.

6-15. *[3]* Let $G = (V, E)$ be an undirected weighted graph, and let T be the shortest-path spanning tree rooted at a vertex v. Suppose now that all the edge weights in G are increased by a constant number k. Is T still the shortest-path spanning tree from v?

6-16. *[3]* Answer all of the following:

(a) Give an example of a weighted connected graph $G = (V, E)$ and a vertex v, such that the minimum spanning tree of G is the same as the shortest-path spanning tree rooted at v.

(b) Give an example of a weighted connected directed graph $G = (V, E)$ and a vertex v, such that the minimum-cost spanning tree of G is very different from the shortest-path spanning tree rooted at v.

(c) Can the two trees be completely disjointed?

6-17. *[3]* Either prove the following or give a counterexample:

(a) Is the path between a pair of vertices in a minimum spanning tree of an undirected graph necessarily the shortest (minimum weight) path?

(b) Suppose that the minimum spanning tree of the graph is unique. Is the path between a pair of vertices in a minimum spanning tree of an undirected graph necessarily the shortest (minimum weight) path?

6-18. *[5]* In certain graph problems, vertices have can have weights instead of or in addition to the weights of edges. Let C_v be the cost of vertex v, and $C_{(x,y)}$ the cost of the edge (x, y). This problem is concerned with finding the cheapest path between vertices a and b in a graph G. The cost of a path is the sum of the costs of the edges and vertices encountered on the path.

(a) Suppose that each edge in the graph has a weight of zero (while non-edges have a cost of ∞). Assume that $C_v = 1$ for all vertices $1 \leq v \leq n$ (i.e. , all vertices have the same cost). Give an *efficient* algorithm to find the cheapest path from a to b and its time complexity.

(b) Now suppose that the vertex costs are not constant (but are all positive) and the edge costs remain as above. Give an *efficient* algorithm to find the cheapest path from a to b and its time complexity.

(c) Now suppose that both the edge and vertex costs are not constant (but are all positive). Give an *efficient* algorithm to find the cheapest path from a to b and its time complexity.

6-19. *[5]* Let G be a weighted *directed* graph with n vertices and m edges, where all edges have positive weight. A directed cycle is a directed path that starts and ends at the same vertex and contains at least one edge. Give an $O(n^3)$ algorithm to find a directed cycle in G of minimum total weight. Partial credit will be given for an $O(n^2 m)$ algorithm.

6-20. *[5]* Can we modify Dijkstra's algorithm to solve the single-source *longest* path problem by changing *minimum* to *maximum*? If so, then prove your algorithm correct. If not, then provide a counterexample.

6-21. *[5]* Let $G = (V, E)$ be a weighted acyclic directed graph with possibly negative edge weights. Design a linear-time algorithm to solve the single-source shortest-path problem from a given source v.

6-22. *[5]* Let $G = (V, E)$ be a directed weighted graph such that all the weights are positive. Let v and w be two vertices in G and $k \leq |V|$ be an integer. Design an algorithm to find the shortest path from v to w that contains exactly k edges. Note that the path need not be simple.

6-23. *[5] Arbitrage* is the use of discrepancies in currency-exchange rates to make a profit. For example, there may be a small window of time during which 1 U.S. dollar buys 0.75 British pounds, 1 British pound buys 2 Australian dollars, and 1 Australian dollar buys 0.70 U.S. dollars. At such a time, a smart trader can trade one U.S. dollar and end up with $0.75 \times 2 \times 0.7 = 1.05$ U.S. dollars—a profit of 5%. Suppose that there are n currencies $c_1, ..., c_n$ and an $n \times n$ table R of exchange rates, such that one unit of currency c_i buys $R[i, j]$ units of currency c_j. Devise and analyze an algorithm to determine the maximum value of

$$R[c_1, c_{i1}] \cdot R[c_{i1}, c_{i2}] \cdots R[c_{ik-1}, c_{ik}] \cdot R[c_{ik}, c_1]$$

Hint: think all-pairs shortest path.

Network Flow and Matching

6-24. *[3]* A matching in a graph is a set of disjoint edges—i.e., edges that do not share any vertices in common. Give a linear-time algorithm to find a maximum matching in a tree.

6-25. *[5]* An *edge cover* of an undirected graph $G = (V, E)$ is a set of edges such that each vertex in the graph is incident to at least one edge from the set. Give an efficient algorithm, based on matching, to find the minimum-size edge cover for G.

Programming Challenges

These programming challenge problems with robot judging are available at *http://www.programming-challenges.com* or *http://online-judge.uva.es*.

6-1. "Freckles" – Programming Challenges 111001, UVA Judge 10034.

6-2. "Necklace" – Programming Challenges 111002, UVA Judge 10054.

6-3. "Railroads" – Programming Challenges 111004, UVA Judge 10039.

6-4. "Tourist Guide" – Programming Challenges 111006, UVA Judge 10199.

6-5. "The Grand Dinner" – Programming Challenges 111007, UVA Judge 10249.

7

Combinatorial Search and Heuristic Methods

We can solve many problems to optimality using exhaustive search techniques, although the time complexity can be enormous. For certain applications, it may pay to spend extra time to be certain of the optimal solution. A good example occurs in testing a circuit or a program on all possible inputs. You can prove the correctness of the device by trying all possible inputs and verifying that they give the correct answer. Verifying correctness is a property to be proud of. However, claiming that it works correctly on all the inputs you tried is worth much less.

Modern computers have clock rates of a few *gigahertz*, meaning billions of operations per second. Since doing something interesting takes a few hundred instructions, you can hope to search millions of items per second on contemporary machines.

It is important to realize how big (or how small) one million is. One million permutations means all arrangements of roughly 10 or 11 objects, but not more. One million subsets means all combinations of roughly 20 items, but not more. Solving significantly larger problems requires carefully pruning the search space to ensure we look at only the elements that really matter.

In this section, we introduce backtracking as a technique for listing all possible solutions for a combinatorial algorithm problem. We illustrate the power of clever pruning techniques to speed up real search applications. For problems that are too large to contemplate using brute-force combinatorial search, we introduce heuristic methods such as simulated annealing. Such heuristic methods are important weapons in any practical algorist's arsenal.

S.S. Skiena, *The Algorithm Design Manual*, 2nd ed., DOI: 10.1007/978-1-84800-070-4_7,
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7.1 Backtracking

Backtracking is a systematic way to iterate through all the possible configurations of a search space. These configurations may represent all possible arrangements of objects (permutations) or all possible ways of building a collection of them (subsets). Other situations may demand enumerating all spanning trees of a graph, all paths between two vertices, or all possible ways to partition vertices into color classes.

What these problems have in common is that we must generate each one possible configuration exactly once. Avoiding both repetitions and missing configurations means that we must define a systematic generation order. We will model our combinatorial search solution as a vector $a = (a_1, a_2, ..., a_n)$, where each element a_i is selected from a finite ordered set S_i. Such a vector might represent an arrangement where a_i contains the ith element of the permutation. Or, the vector might represent a given subset S, where a_i is true if and only if the ith element of the universe is in S. The vector can even represent a sequence of moves in a game or a path in a graph, where a_i contains the ith event in the sequence.

At each step in the backtracking algorithm, we try to extend a given partial solution $a = (a_1, a_2, ..., a_k)$ by adding another element at the end. After extending it, we must test whether what we now have is a solution: if so, we should print it or count it. If not, we must check whether the partial solution is still potentially extendible to some complete solution.

Backtracking constructs a tree of partial solutions, where each vertex represents a partial solution. There is an edge from x to y if node y was created by advancing from x. This tree of partial solutions provides an alternative way to think about backtracking, for the process of constructing the solutions corresponds exactly to doing a depth-first traversal of the backtrack tree. Viewing backtracking as a depth-first search on an implicit graph yields a natural recursive implementation of the basic algorithm.

```
Backtrack-DFS(A, k)
    if A = (a_1, a_2, ..., a_k) is a solution, report it.
    else
        k = k + 1
        compute S_k
        while S_k ≠ ∅ do
            a_k = an element in S_k
            S_k = S_k − a_k
            Backtrack-DFS(A, k)
```

Although a breadth-first search could also be used to enumerate solutions, a depth-first search is greatly preferred because it uses much less space. The current state of a search is completely represented by the path from the root to the current search depth-first node. This requires space proportional to the *height* of the tree. In breadth-first search, the queue stores all the nodes at the current level, which

is proportional to the *width* of the search tree. For most interesting problems, the width of the tree grows exponentially in its height.

Implementation

The honest working `backtrack` code is given below:

```
bool finished = FALSE;            /* found all solutions yet? */

backtrack(int a[], int k, data input)
{
     int c[MAXCANDIDATES];     /* candidates for next position */
     int ncandidates;          /* next position candidate count */
     int i;                    /* counter */

     if (is_a_solution(a,k,input))
             process_solution(a,k,input);
     else {
             k = k+1;
             construct_candidates(a,k,input,c,&ncandidates);
             for (i=0; i<ncandidates; i++) {
                     a[k] = c[i];
                     make_move(a,k,input);
                     backtrack(a,k,input);
                     unmake_move(a,k,input);
                     if (finished) return;   /* terminate early */
             }
     }
}
```

Backtracking ensures correctness by enumerating all possibilities. It ensures efficiency by never visiting a state more than once.

Study how recursion yields an elegant and easy implementation of the backtracking algorithm. Because a new candidates array `c` is allocated with each recursive procedure call, the subsets of not-yet-considered extension candidates at each position will not interfere with each other.

The application-specific parts of this algorithm consists of five subroutines:

- `is_a_solution(a,k,input)` – This Boolean function tests whether the first k elements of vector a from a complete solution for the given problem. The last argument, `input`, allows us to pass general information into the routine. We can use it to specify n—the size of a target solution. This makes sense when constructing permutations or subsets of n elements, but other data may be relevant when constructing variable-sized objects such as sequences of moves in a game.

- `construct_candidates(a,k,input,c,ncandidates)` – This routine fills an array c with the complete set of possible candidates for the kth position of a, given the contents of the first $k-1$ positions. The number of candidates returned in this array is denoted by `ncandidates`. Again, `input` may be used to pass auxiliary information.

- `process_solution(a,k,input)` – This routine prints, counts, or however processes a complete solution once it is constructed.

- `make_move(a,k,input)` *and* `unmake_move(a,k,input)` – These routines enable us to modify a data structure in response to the latest move, as well as clean up this data structure if we decide to take back the move. Such a data structure could be rebuilt from scratch from the solution vector a as needed, but this is inefficient when each move involves incremental changes that can easily be undone.

  These calls function as null stubs in all of this section's examples, but will be employed in the Sudoku program of Section 7.3 (page 239).

We include a global `finished` flag to allow for premature termination, which could be set in any application-specific routine.

To really understand how backtracking works, you must see how such objects as permutations and subsets can be constructed by defining the right state spaces. Examples of several state spaces are described in subsections below.

7.1.1 Constructing All Subsets

A critical issue when designing state spaces to represent combinatorial objects is how many objects need representing. How many subsets are there of an n-element set, say the integers $\{1, \ldots, n\}$? There are exactly two subsets for $n = 1$, namely $\{\}$ and $\{1\}$. There are four subsets for $n = 2$, and eight subsets for $n = 3$. Each new element doubles the number of possibilities, so there are 2^n subsets of n elements.

Each subset is described by elements that are in it. To construct all 2^n subsets, we set up an array/vector of n cells, where the value of a_i (true or false) signifies whether the ith item is in the given subset. In the scheme of our general backtrack algorithm, $S_k = (true, false)$ and a is a solution whenever $k = n$. We can now construct all subsets with simple implementations of `is_a_solution()`, `construct_candidates()`, and `process_solution()`.

```
is_a_solution(int a[], int k, int n)
{
        return (k == n);                /* is k == n? */
}
```

```
construct_candidates(int a[], int k, int n, int c[], int *ncandidates)
{
        c[0] = TRUE;
        c[1] = FALSE;
        *ncandidates = 2;
}


process_solution(int a[], int k)
{
        int i;                          /* counter */

        printf("{");
        for (i=1; i<=k; i++)
                if (a[i] == TRUE) printf(" %d",i);

        printf(" }\n");
}
```

Printing each out subset after constructing it proves to be the most complicated of the three routines!

Finally, we must instantiate the call to `backtrack` with the right arguments. Specifically, this means giving a pointer to the empty solution vector, setting $k = 0$ to denote that it is empty, and specifying the number of elements in the universal set:

```
generate_subsets(int n)
{
        int a[NMAX];                    /* solution vector */

        backtrack(a,0,n);
}
```

In what order will the subsets of $\{1, 2, 3\}$ be generated? It depends on the order of moves `construct_candidates`. Since *true* always appears before *false*, the subset of all trues is generated first, and the all-false empty set is generated last: {123}, {12}, {13}, {1}, {23}, {2}, {3}, {}

Trace through this example carefully to make sure you understand the backtracking procedure. The problem of generating subsets is more thoroughly discussed in Section 14.5 (page 452).

7.1.2 Constructing All Permutations

Counting permutations of $\{1, \ldots, n\}$ is a necessary prerequisite to generating them. There are n distinct choices for the value of the first element of a permutation. Once

we have fixed a_1, there are $n-1$ candidates remaining for the second position, since we can have any value except a_1 (repetitions are forbidden in permutation). Repeating this argument yields a total of $n! = \prod_{i=1}^{n} i$ distinct permutations.

This counting argument suggests a suitable representation. Set up an array/vector a of n cells. The set of candidates for the ith position will be the set of elements that have not appeared in the $(i-1)$ elements of the partial solution, corresponding to the first $i-1$ elements of the permutation.

In the scheme of the general backtrack algorithm, $S_k = \{1, \ldots, n\} - a$, and a is a solution whenever $k = n$:

```
construct_candidates(int a[], int k, int n, int c[], int *ncandidates)
{
        int i;                          /* counter */
        bool in_perm[NMAX];             /* who is in the permutation? */

        for (i=1; i<NMAX; i++) in_perm[i] = FALSE;
        for (i=0; i<k; i++) in_perm[ a[i] ] = TRUE;

        *ncandidates = 0;
        for (i=1; i<=n; i++)
                if (in_perm[i] == FALSE) {
                        c[ *ncandidates] = i;
                        *ncandidates = *ncandidates + 1;
                }
}
```

Testing whether i is a candidate for the kth slot in the permutation can be done by iterating through all $k-1$ elements of a and verifying that none of them matched. However, we prefer to set up a bit-vector data structure (see Section 12.5 (page 385)) to maintain which elements are in the partial solution. This gives a constant-time legality check.

Completing the job requires specifying `process_solution` and `is_a_solution`, as well as setting the appropriate arguments to `backtrack`. All are essentially the same as for subsets:

```
process_solution(int a[], int k)
{
        int i;                          /* counter */

        for (i=1; i<=k; i++) printf(" %d",a[i]);

        printf("\n");
}
```

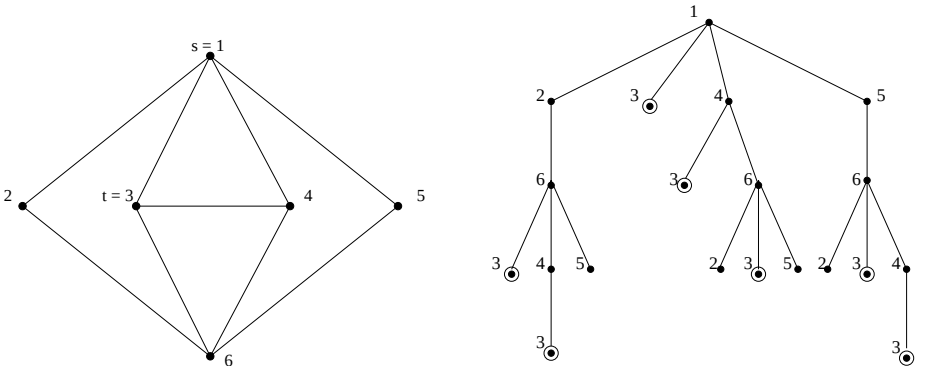

Figure 7.1: Search tree enumerating all simple s-t paths in the given graph (left).

```
is_a_solution(int a[], int k, int n)
{
        return (k == n);
}


generate_permutations(int n)
{
        int a[NMAX];                    /* solution vector */

        backtrack(a,0,n);
}
```

As a consequence of the candidate order, these routines generate permutations in *lexicographic*, or sorted order—i.e., `123`, `132`, `213`, `231`, `312`, and `321`. The problem of generating permutations is more thoroughly discussed in Section 14.4 (page 448).

7.1.3 Constructing All Paths in a Graph

Enumerating all the simple s to t paths through a given graph is a more complicated problem than listing permutations or subsets. There is no explicit formula that counts the number of solutions as a function of the number of edges or vertices, because the number of paths depends upon the structure of the graph.

The starting point of any path from s to t is always s. Thus, s is the only candidate for the first position and $S_1 = \{s\}$. The possible candidates for the second position are the vertices v such that (s, v) is an edge of the graph, for the path wanders from vertex to vertex using edges to define the legal steps. In general,

S_{k+1} consists of the set of vertices adjacent to a_k that have not been used elsewhere in the partial solution A.

```
construct_candidates(int a[], int k, int n, int c[], int *ncandidates)
{
     int i;                    /* counters */
     bool in_sol[NMAX];        /* what's already in the solution? */
     edgenode *p;              /* temporary pointer */
     int last;                 /* last vertex on current path */

     for (i=1; i<NMAX; i++) in_sol[i] = FALSE;
     for (i=1; i<k; i++) in_sol[ a[i] ] = TRUE;

     if (k==1) {               /* always start from vertex 1 */
             c[0] = 1;
             *ncandidates = 1;
     }
     else    {
             *ncandidates = 0;
             last = a[k-1];
             p = g.edges[last];
             while (p != NULL) {
                     if (!in_sol[ p->y ]) {
                             c[*ncandidates] = p->y;
                             *ncandidates = *ncandidates + 1;
                     }
                     p = p->next;
             }
     }
}
```

We report a successful path whenever $a_k = t$.

```
is_a_solution(int a[], int k, int t)
{
        return (a[k] == t);
}

process_solution(int a[], int k)
{
        solution_count ++;        /* count all s to t paths */
}
```

The solution vector A must have room for all n vertices, although most paths are likely shorter than this. Figure 7.1 shows the search tree giving all paths from a particular vertex in an example graph.

7.2 Search Pruning

Backtracking ensures correctness by enumerating all possibilities. Enumerating all $n!$ permutations of n vertices of the graph and selecting the best one yields the correct algorithm to find the optimal traveling salesman tour. For each permutation, we could see whether all edges implied by the tour really exists in the graph G, and if so, add the weights of these edges together.

However, it would be wasteful to construct all the permutations first and then analyze them later. Suppose our search started from vertex v_1, and it happened that edge (v_1, v_2) was not in G. The next $(n-2)!$ permutations enumerated starting with (v_1, v_2) would be a complete waste of effort. Much better would be to prune the search after v_1, v_2 and continue next with v_1, v_3. By restricting the set of next elements to reflect only moves that are legal from the current partial configuration, we significantly reduce the search complexity.

Pruning is the technique of cutting off the search the instant we have established that a partial solution cannot be extended into a full solution. For traveling salesman, we seek the cheapest tour that visits all vertices. Suppose that in the course of our search we find a tour t whose cost is C_t. Later, we may have a partial solution a whose edge sum $C_A > C_t$. Is there any reason to continue exploring this node? No, because any tour with this prefix $a_1, \ldots, a_k$ will have cost greater than tour t, and hence is doomed to be nonoptimal. Cutting away such failed partial tours as soon as possible can have an enormous impact on running time.

Exploiting symmetry is another avenue for reducing combinatorial searches. Pruning away partial solutions identical to those previously considered requires recognizing underlying symmetries in the search space. For example, consider the state of our TSP search after we have tried all partial positions beginning with v_1. Does it pay to continue the search with partial solutions beginning with v_2? No. Any tour starting and ending at v_2 can be viewed as a rotation of one starting and ending at v_1, for these tours are cycles. There are thus only $(n-1)!$ distinct tours on n vertices, not $n!$. By restricting the first element of the tour to v_1, we save a factor of n in time without missing any interesting solutions. Detecting such symmetries can be subtle, but once identified they can usually be easily exploited.

> *Take-Home Lesson:* Combinatorial searches, when augmented with tree pruning techniques, can be used to find the optimal solution of small optimization problems. How small depends upon the specific problem, but typical size limits are somewhere between $15 \leq n \leq 50$ items.

		1 2
	3 5	
6		7
7		3
	4	8
1		
	1 2	
8		4
5		6

6	7	3	8	9	4	5	1	2
9	1	2	7	3	5	4	8	6
8	4	5	6	1	2	9	7	3
7	9	8	2	6	1	3	5	4
5	2	6	4	7	3	8	9	1
1	3	4	5	8	9	2	6	7
4	6	9	1	2	8	7	3	5
2	8	7	3	5	6	1	4	9
3	5	1	9	4	7	6	2	8

Figure 7.2: Challenging Sudoku puzzle (l) with solution (r)

7.3 Sudoku

A Sudoku craze has swept the world. Many newspapers now publish daily Sudoku puzzles, and millions of books about Sudoku have been sold. British Airways sent a formal memo forbidding its cabin crews from doing Sudoku during takeoffs and landings. Indeed, I have noticed plenty of Sudoku going on in the back of my algorithms classes during lecture.

What is Sudoku? In its most common form, it consists of a 9×9 grid filled with blanks and the digits 1 to 9. The puzzle is completed when every row, column, and sector (3×3 subproblems corresponding to the nine sectors of a tic-tac-toe puzzle) contain the digits 1 through 9 with no deletions or repetition. Figure 7.2 presents a challenging Sudoku puzzle and its solution.

Backtracking lends itself nicely to the problem of solving Sudoku puzzles. We will use the puzzle here to better illustrate the algorithmic technique. Our state space will be the sequence of open squares, each of which must ultimately be filled in with a number. The candidates for open squares (i, j) are exactly the integers from 1 to 9 that have not yet appeared in row i, column j, or the 3×3 sector containing (i, j). We backtrack as soon as we are out of candidates for a square.

The solution vector `a` supported by `backtrack` only accepts a single integer per position. This is enough to store contents of a board square (1-9) but not the coordinates of the board square. Thus, we keep a separate array of `move` positions as part of our `board` data type provided below. The basic data structures we need to support our solution are:

```
#define DIMENSION 9                  /* 9*9 board */
#define NCELLS  DIMENSION*DIMENSION /* 81 cells in a 9*9 problem */

typedef struct {
    int x, y;                        /* x and y coordinates of point */
} point;
```

```
typedef struct {
    int m[DIMENSION+1][DIMENSION+1]; /* matrix of board contents */
    int freecount;                   /* how many open squares remain? */
    point move[NCELLS+1];            /* how did we fill the squares? */
} boardtype;
```

Constructing the candidates for the next solution position involves first picking the open square we want to fill next (`next_square`), and then identifying which numbers are candidates to fill that square (`possible_values`). These routines are basically bookkeeping, although the subtle details of how they work can have an enormous impact on performance.

```
construct_candidates(int a[], int k, boardtype *board, int c[],
                     int *ncandidates)
{
   int x,y;                     /* position of next move */
   int i;                       /* counter */
   bool possible[DIMENSION+1]; /* what is possible for the square */

   next_square(&x,&y,board);   /* which square should we fill next? */

   board->move[k].x = x;       /* store our choice of next position */
   board->move[k].y = y;

   *ncandidates = 0;

   if ((x<0) && (y<0)) return; /* error condition, no moves possible */

   possible_values(x,y,board,possible);
   for (i=0; i<=DIMENSION; i++)
           if (possible[i] == TRUE) {
                   c[*ncandidates] = i;
                   *ncandidates = *ncandidates + 1;
           }
}
```

We must update our `board` data structure to reflect the effect of filling a candidate value into a square, as well as remove these changes should we backtrack away from this position. These updates are handled by `make_move` and `unmake_move`, both of which are called directly from `backtrack`:

```
make_move(int a[], int k, boardtype *board)
{
        fill_square(board->move[k].x,board->move[k].y,a[k],board);
}


unmake_move(int a[], int k, boardtype *board)
{
        free_square(board->move[k].x,board->move[k].y,board);
}
```

One important job for these board update routines is maintaining how many free squares remain on the board. A solution is found when there are no more free squares remaining to be filled:

```
is_a_solution(int a[], int k, boardtype *board)
{
        if (board->freecount == 0)
                return (TRUE);
        else
                return(FALSE);
}
```

We print the configuration and turn off the backtrack search by setting off the global `finished` flag on finding a solution. This can be done without consequence because "official" Sudoku puzzles are only allowed to have one solution. There can be an enormous number of solutions to nonofficial Sudoku puzzles. Indeed, the empty puzzle (where no number is initially specified) can be filled in exactly 6,670,903,752,021,072,936,960 ways. We can ensure we don't see all of them by turning off the search:

```
process_solution(int a[], int k, boardtype *board)
{
        print_board(board);
        finished = TRUE;
}
```

This completes the program modulo details of identifying the next open square to fill (`next_square`) and identifying the candidates to fill that square (`possible_values`). Two reasonable ways to select the next square are:

- *Arbitrary Square Selection* – Pick the first open square we encounter, possibly picking the first, the last, or a random open square. All are equivalent in that there seems to be no reason to believe that one heuristic will perform any better than the other.

- *Most Constrained Square Selection* – Here, we check each of the open squares (i, j) to see how many number candidates remain for each—i.e. , have not already been used in either row i, column j, or the sector containing (i, j). We pick the square with the fewest number of candidates.

Although both possibilities work correctly, the second option is much, much better. Often there will be open squares with only one remaining candidate. For these, the choice is forced. We might as well make it now, especially since pinning this value down will help trim the possibilities for other open squares. Of course, we will spend more time selecting each candidate square, but if the puzzle is easy enough we may never have to backtrack at all.

If the most constrained square has two possibilities, we have a 1/2 probability of guessing right the first time, as opposed to a $(1/9)^{th}$ probability for a completely unconstrained square. Reducing our average number of choices from (say) 3 per square to 2 per square is an enormous win, since it multiplies for each position. If we have (say) 20 positions to fill, we must enumerate only $2^{20} = 1,048,576$ solutions. A branching factor of 3 at each of the 20 positions will result in over $3,000$ times as much work!

Our final decision concerns the `possible_values` we allow for each square. We have two possibilities:

- *Local Count* – Our backtrack search works correctly if the routine generating candidates for board position (i, j) (`possible_values`) does the obvious thing and allows all numbers 1 to 9 that have not appeared in the given row, column, or sector.

- *Look ahead* – But what if our current partial solution has some *other* open square where there are no candidates remaining under the local count criteria? There is no possible way to complete this partial solution into a full Sudoku grid. Thus there *really* are zero possible moves to consider for (i, j) because of what is happening elsewhere on the board!

  We will discover this obstruction eventually, when we pick this square for expansion, discover it has no moves, and then have to backtrack. But why wait, since all our efforts until then will be wasted? We are *much* better off backtracking immediately and moving on.[1]

Successful pruning requires looking ahead to see when a solution is doomed to go nowhere, and backing off as soon as possible.

Table 7.1 presents the number of calls to `is_a_solution` for all four backtracking variants on three Sudoku instances of varying complexity:

[1]This look-ahead condition might have naturally followed from the most-constrained square selection, had it been permitted to select squares with no moves. However, my implementation credited squares that already contained numbers as having no moves, thus limiting the next square choices to squares with at least one move.

Pruning Condition		Puzzle Complexity		
`next_square`	`possible_values`	Easy	Medium	Hard
arbitrary	local count	1,904,832	863,305	never finished
arbitrary	look ahead	127	142	12,507,212
most constrained	local count	48	84	1,243,838
most constrained	look ahead	48	65	10,374

Table 7.1: Sudoku run times (in number of steps) under different pruning strategies

- The *Easy* board was intended to be easy for a human player. Indeed, my program solved it without any backtracking steps when the most constrained square was selected as the next position.
- The *Medium* board stumped all the contestants at the finals of the World Sudoku Championship in March 2006. The decent search variants still required only a few backtrack steps to dispatch this problem.
- The *Hard* problem is the board displayed in Figure 7.2, which contains only 17 fixed numbers. This is the fewest specified known number of positions in any problem instance that has only one complete solution.

What is considered to be a "hard" problem instance depends upon the given heuristic. Certainly you know people who find math/theory harder than programming and others who think differently. Heuristic A may well think instance I_1 is easier than I_2, while heuristic B ranks them in the other order.

What can we learn from these experiments? Looking ahead to eliminate dead positions as soon as possible is the best way to prune a search. Without this operation, we never finished the hardest puzzle and took thousands of times longer than we should have on the easier ones.

Smart square selection had a similar impact, even though it nominally just rearranges the order in which we do the work. However, doing more constrained positions first is tantamount to reducing the outdegree of each node in the tree, and each additional position we fix adds constraints that help lower the degree for future selections.

It took the better part of an hour (48:44) to solve the puzzle in Figure 7.2 when I selected an arbitrary square for my next move. Sure, my program was faster in most instances, but Sudoku puzzles are designed to be solved by people using pencils in much less time than this. Making the next move in the most constricted square reduced search time by a factor of over 1,200. Each puzzle we tried can now be solved in seconds—the time it takes to reach for the pencil if you want to do it by hand.

This is the power of a pruning search. Even simple pruning strategies can suffice to reduce running time from impossible to instantaneous.

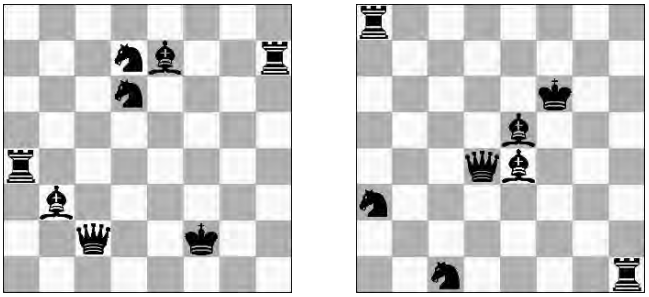

Figure 7.3: Configurations covering 63 but not 64 squares

7.4 War Story: Covering Chessboards

Every researcher dreams of solving a classical problem—one that has remained open and unsolved for over a century. There is something romantic about communicating across the generations, being part of the evolution of science, and helping to climb another rung up the ladder of human progress. There is also a pleasant sense of smugness that comes from figuring out how to do something that nobody could do before you.

There are several possible reasons why a problem might stay open for such a long period of time. Perhaps it is so difficult and profound that it requires a uniquely powerful intellect to solve. A second reason is technological—the ideas or techniques required to solve the problem may not have existed when it was first posed. A final possibility is that no one may have cared enough about the problem in the interim to seriously bother with it. Once, I helped solve a problem that had been open for over a hundred years. Decide for yourself which reason best explains why.

Chess is a game that has fascinated mankind for thousands of years. In addition, it has inspired many combinatorial problems of independent interest. The combinatorial explosion was first recognized with the legend that the inventor of chess demanded as payment one grain of rice for the first square of the board, and twice as much for the $(i+1)$st square than the ith square. The king was astonished to learn he had to cough up $\sum_{i=1}^{64} 2^i = 2^{65} - 1 = 36{,}893{,}488{,}147{,}419{,}103{,}231$ grains of rice. In beheading the inventor, the wise king first established pruning as a technique for dealing with the combinatorial explosion.

In 1849, Kling posed the question of whether all 64 squares on the board can be simultaneously threatened by an arrangement of the eight main pieces on the chess board—the king, queen, two knights, two rooks, and two oppositely colored bishops. Pieces do not threaten the square they sit on. Configurations that simultaneously threaten 63 squares, such as those in Figure 7.3, have been known for a long time, but whether this was the best possible remained an open problem. This problem

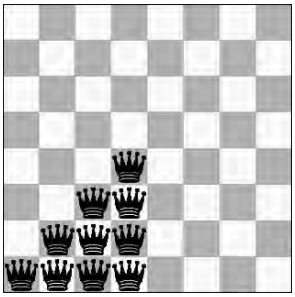

Figure 7.4: The ten unique positions for the queen, with respect to symmetry

seemed ripe for solution by exhaustive combinatorial searching, although whether it was solvable depended upon the size of the search space.

Consider the eight main pieces in chess (king, queen, two rooks, two bishops, and two knights). How many ways can they be positioned on a chessboard? The trivial bound is $64!/(64-8)! = 178{,}462{,}987{,}637{,}760 \approx 10^{15}$ positions. Anything much larger than about 10^9 positions would be unreasonable to search on a modest computer in a modest amount of time.

Getting the job done would require significant pruning. Our first idea was to remove symmetries. Accounting for orthogonal and diagonal symmetries left only ten distinct positions for the queen, shown in Figure 7.4.

Once the queen is placed, there are $64 \cdot 63/2 = 2{,}016$ distinct ways to position a pair of rooks or knights, 64 places to locate the king, and 32 spots for each of the white and black bishops. Such an exhaustive search would test $2{,}663{,}550{,}812{,}160 \approx 10^{13}$ distinct positions—still much too large to try.

We could use backtracking to construct all of the positions, but we had to find a way to prune the search space significantly. Pruning the search meant that we needed a quick way to prove that there was no way to complete a partially filled-in position to cover all 64 squares. Suppose we had already placed seven pieces on the board, and together they covered all but 10 squares of the board. Say the remaining piece was the king. Can there be a position to place the king so that all squares are threatened? The answer must be no, because the king can threaten at most eight squares according to the rules of chess. There can be no reason to test any king position. We might win big pruning such configurations.

This pruning strategy required carefully ordering the evaluation of the pieces. Each piece can threaten a certain maximum number of squares: the queen 27, the king/knight 8, the rook 14, and the bishop 13. We would want to insert the pieces in decreasing order of mobility. We can prune when the number of unthreatened squares exceeds the sum of the maximum coverage of the unplaced pieces. This sum is minimized by using the decreasing order of mobility.

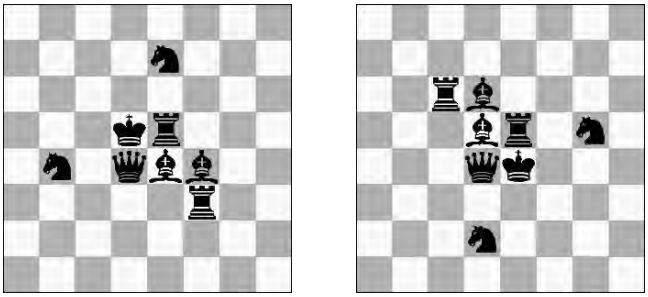

Figure 7.5: Weakly covering 64 squares

When we implemented a backtrack search using this pruning strategy, we found that it eliminated over 95% of the search space. After optimizing our move generation, our program could search over 1,000 positions per second. But this was still too slow, for $10^{12}/10^3 = 10^9$ seconds meant 1,000 days! Although we might further tweak the program to speed it up by an order of magnitude or so, what we really needed was to find a way to prune more nodes.

Effective pruning meant eliminating large numbers of positions at a single stroke. Our previous attempt was too weak. What if instead of placing up to eight pieces on the board simultaneously, we placed *more* than eight pieces. Obviously, the more pieces we placed simultaneously, the more likely they would threaten all 64 squares. But *if* they didn't cover, all subsets of eight distinct pieces from the set couldn't possibly threaten all squares. The potential existed to eliminate a vast number of positions by pruning a single node.

So in our final version, the nodes of our search tree corresponded to chessboards that could have any number of pieces, and more than one piece on a square. For a given board, we distinguished *strong* and *weak* attacks on a square. A strong attack corresponds to the usual notion of a threat in chess. A square is *weakly attacked* if the square is strongly attacked by some subset of the board—that is, a weak attack ignores any possible blocking effects of intervening pieces. All 64 squares can be weakly attacked with eight pieces, as shown in Figure 7.5.

Our algorithm consisted of two passes. The first pass listed boards where every square was weakly attacked. The second pass filtered the list by considering blocking pieces. A weak attack is much faster to compute (no blocking to worry about), and any strong attack set is always a subset of a weak attack set. The position could be pruned whenever there was a non-weakly threatened square.

This program was efficient enough to complete the search on a slow 1988-era IBM PC-RT in under one day. It did not find a single position covering all 64 squares with the bishops on opposite colored squares. However, our program showed that it is possible to cover the board with *seven* pieces provided a queen and a knight can occupy the same square, as shown in Figure 7.6.

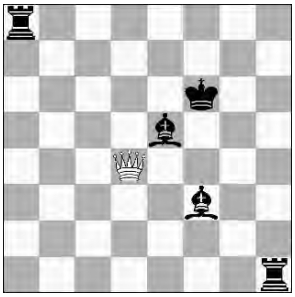

Figure 7.6: Seven pieces suffice when superimposing queen and knight (shown as a white queen)

Take-Home Lesson: Clever pruning can make short work of surprisingly hard combinatorial search problems. Proper pruning will have a greater impact on search time than any other factor.

7.5 Heuristic Search Methods

Heuristic methods provide an alternate way to approach difficult combinatorial optimization problems. Backtracking gave us a method to find the best of all possible solutions, as scored by a given objective function. However, any algorithm searching all configurations is doomed to be impossible on large instances.

In this section, we discuss such heuristic search methods. We devote the bulk of our attention to simulated annealing, which I find to be the most reliable method to apply in practice. Heuristic search algorithms have an air of voodoo about them, but how they work and why one method might work better than another follows logically enough if you think them through.

In particular, we will look at three different heuristic search methods: random sampling, gradient-descent search, and simulated annealing. The traveling salesman problem will be our ongoing example for comparing heuristics. All three methods have two common components:

- *Solution space representation* – This is a complete yet concise description of the set of possible solutions for the problem. For traveling salesman, the solution space consists of $(n-1)!$ elements—namely all possible circular permutations of the vertices. We need a data structure to represent each element of the solution space. For TSP, the candidate solutions can naturally be represented using an array S of $n-1$ vertices, where S_i defines the $(i+1)$st vertex on the tour starting from v_1.
- *Cost function* – Search methods need a *cost* or *evaluation* function to access the quality of each element of the solution space. Our search heuristic

identifies the element with the best possible score—either highest or lowest depending upon the nature of the problem. For TSP, the cost function for evaluating a given candidate solution S should just sum up the costs involved, namely the weight of all edges (S_i, S_{i+1}), where S_{n+1} denotes v_1.

7.5.1 Random Sampling

The simplest method to search in a solution space uses random sampling. It is also called the *Monte Carlo method*. We repeatedly construct random solutions and evaluate them, stopping as soon as we get a good enough solution, or (more likely) when we are tired of waiting. We report the best solution found over the course of our sampling.

True random sampling requires that we are able to select elements from the solution space *uniformly at random*. This means that each of the elements of the solution space must have an equal probability of being the next candidate selected. Such sampling can be a subtle problem. Algorithms for generating random permutations, subsets, partitions, and graphs are discussed in Sections 14.4-14.7.

```
random_sampling(tsp_instance *t, int nsamples, tsp_solution *bestsol)
{
        tsp_solution s;                 /* current tsp solution */
        double best_cost;               /* best cost so far */
        double cost_now;                /* current cost */
        int i;                          /* counter */

        initialize_solution(t->n,&s);
        best_cost = solution_cost(&s,t);
        copy_solution(&s,bestsol);

        for (i=1; i<=nsamples; i++) {
                random_solution(&s);
                cost_now = solution_cost(&s,t);
                if (cost_now < best_cost) {
                        best_cost = cost_now;
                        copy_solution(&s,bestsol);
                }
        }
}
```

When might random sampling do well?

- *When there are a high proportion of acceptable solutions* – Finding a piece of hay in a haystack is easy, since almost anything you grab is a straw. When solutions are plentiful, a random search should find one quickly.

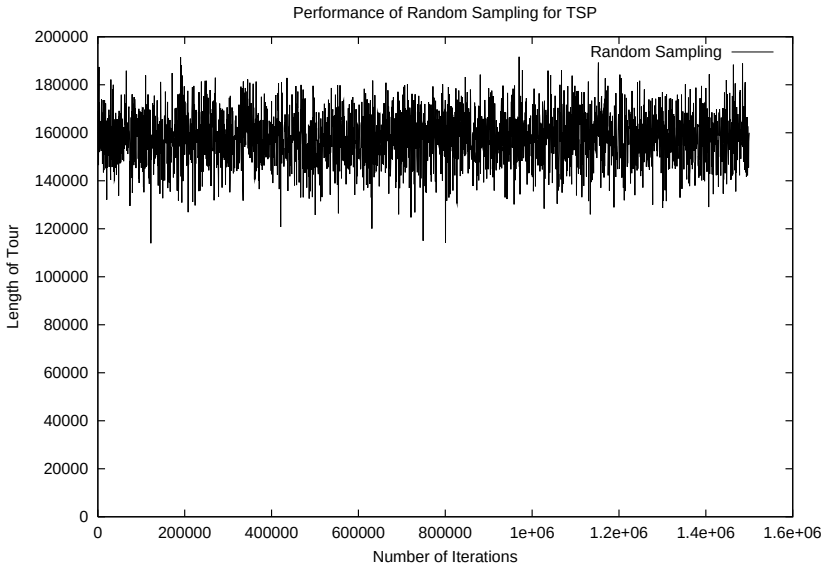

Figure 7.7: Search time/quality tradeoffs for TSP using random sampling.

Finding prime numbers is domain where a random search proves successful. Generating large random prime numbers for keys is an important aspect of cryptographic systems such as RSA. Roughly one out of every $\ln n$ integers are prime, so only a modest number of samples need to be taken to discover primes that are several hundred digits long.

- *When there is no coherence in the solution space* – Random sampling is the right thing to do when there is no sense of when we are getting *closer* to a solution. Suppose you wanted to find one of your friends who has a social security number that ends in 00. There is not much you can hope to do but tap an arbitrary fellow on their shoulder and ask. No cleverer method will be better than random sampling.

  Consider again the problem of hunting for a large prime number. Primes are scattered quite arbitrarily among the integers. Random sampling is as good as anything else.

How does random sampling do on TSP? Pretty lousy. The best solution I found after testing 1.5 million random permutations of a classic TSP instance (the capital cities of the 48 continental United States) was 101,712.8. This is more than three times the cost of the optimal tour! The solution space consists almost entirely

of mediocre to bad solutions, so quality grows very slowly with the amount of sampling / running time we invest. Figure 7.7 presents the arbitrary up-and-down movements of random sampling and generally poor quality solutions encountered on the journey, so you can get a sense of how the score varied over each iteration.

Most problems we encounter, like TSP, have relatively few good solutions but a highly coherent solution space. More powerful heuristic search algorithms are required to deal effectively with such problems.

Stop and Think: Picking the Pair

Problem: We need an efficient and unbiased way to generate random pairs of vertices to perform random vertex swaps. Propose an efficient algorithm to generate elements from the $\binom{n}{2}$ *unordered* pairs on $\{1, \ldots, n\}$ uniformly at random.

Solution: Uniformly generating random structures is a surprisingly subtle problem. Consider the following procedure to generate random unordered pairs:

```
i = random_int(1,n-1);
j = random_int(i+1,n);
```

It is clear that this indeed generates unordered pairs, since $i < j$. Further, it is clear that all $\binom{n}{2}$ unordered pairs can indeed be generated, assuming that `random_int` generates integers uniformly between its two arguments.

But are they uniform? The answer is no. What is the probability that pair $(1, 2)$ is generated? There is a $1/(n-1)$ chance of getting the 1, and then a $1/(n-1)$ chance of getting the 2, which yields $p(1, 2) = 1/(n-1)^2$. But what is the probability of getting $(n-1, n)$? Again, there is a $1/n$ chance of getting the first number, but now there is only one possible choice for the second candidate! This pair will occur n times more often than the first!

The problem is that fewer pairs start with big numbers than little numbers. We could solve this problem by calculating exactly how unordered pairs start with i (exactly $(n-i)$) and appropriately bias the probability. The second value could then be selected uniformly at random from $i+1$ to n.

But instead of working through the math, let's exploit the fact that randomly generating the n^2 *ordered* pairs uniformly is easy. Just pick two integers independently of each other. Ignoring the ordering (i.e. , permuting the ordered pair to unordered pair (x, y) so that $x < y$) gives us a $2/n^2$ probability of generating each unordered pair of distinct elements. If we happen to generate a pair (x, x), we discard it and try again. We will get unordered pairs uniformly at random in constant expected time using the following algorithm:

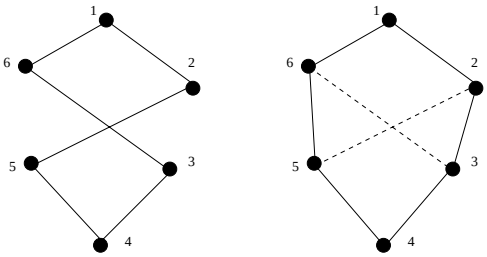

Figure 7.8: Improving a TSP tour by swapping vertices 2 and 6

```
do {
     i = random_int(1,n);
     j = random_int(1,n);
     if (i > j) swap(&i,&j);
} while (i==j);
```

■

7.5.2 Local Search

Now suppose you want to hire an algorithms expert as a consultant to solve your problem. You *could* dial a phone number at random, ask if they are an algorithms expert, and hang up the phone if they say no. After many repetitions you will probably find one, but it would probably be more efficient to ask the fellow on the phone for someone more likely to know an algorithms expert, and call *them* up instead.

A local search employs *local neighborhood* around every element in the solution space. Think of each element x in the solution space as a vertex, with a directed edge (x, y) to every candidate solution y that is a neighbor of x. Our search proceeds from x to the most promising candidate in x's neighborhood.

We certainly do *not* want to explicitly construct this neighborhood graph for any sizable solution space. Think about TSP, which will have $(n-1)!$ vertices in this graph. We are conducting a heuristic search precisely because we cannot hope to do this many operations in a reasonable amount of time.

Instead, we want a general transition mechanism that takes us to the next solution by slightly modifying the current one. Typical transition mechanisms include swapping a random pair of items or changing (inserting or deleting) a single item in the solution.

The most obvious transition mechanism for TSP would be to swap the current tour positions of a random pair of vertices S_i and S_j, as shown in Figure 7.8.

This changes up to eight edges on the tour, deleting the edges currently adjacent to both S_i and S_j, and adding their replacements. Ideally, the effect that these incremental changes have on measuring the quality of the solution can be computed incrementally, so cost function evaluation takes time proportional to the size of the change (typically constant) instead of linear to the size of the solution.

A local search heuristic starts from an arbitrary element of the solution space, and then scans the neighborhood looking for a favorable transition to take. For TSP, this would be *transition*, which lowers the cost of the tour. In a *hill-climbing* procedure, we try to find the top of a mountain (or alternately, the lowest point in a ditch) by starting at some arbitrary point and taking any step that leads in the direction we want to travel. We repeat until we have reached a point where all our neighbors lead us in the wrong direction. We are now *King of the Hill* (or *Dean of the Ditch*).

We are probably not *King of the Mountain*, however. Suppose you wake up in a ski lodge, eager to reach the top of the neighboring peak. Your first transition to gain altitude might be to go upstairs to the top of the building. And then you are trapped. To reach the top of the mountain, you must go downstairs and walk outside, but this violates the requirement that each step has to increase your score. Hill-climbing and closely related heuristics such as greedy search or gradient descent search are great at finding local optima quickly, but often fail to find the globally best solution.

```
hill_climbing(tsp_instance *t, tsp_solution *s)
{
     double cost;                /* best cost so far */
     double delta;               /* swap cost */
     int i,j;                    /* counters */
     bool stuck;                 /* did I get a better solution? */
     double transition();

     initialize_solution(t->n,s);
     random_solution(s);
     cost = solution_cost(s,t);

     do {
             stuck = TRUE;
             for (i=1; i<t->n; i++)
                     for (j=i+1; j<=t->n; j++) {
                             delta = transition(s,t,i,j);
                             if (delta < 0) {
                                     stuck = FALSE;
                                     cost = cost + delta;
                             }
```

```
                        else
                                transition(s,t,j,i);
                    }
    } while (!stuck);
}
```

When does local search do well?

- *When there is great coherence in the solution space* – Hill climbing is at its best when the solution space is *convex*. In other words, it consists of exactly one hill. No matter where you start on the hill, there is always a direction to walk up until you are at the absolute global maximum.

  Many natural problems do have this property. We can think of a binary search as starting in the middle of a search space, where exactly one of the two possible directions we can walk will get us closer to the target key. The simplex algorithm for linear programming (see Section 13.6 (page 411)) is nothing more than hill-climbing over the right solution space, yet guarantees us the optimal solution to any linear programming problem.

- *Whenever the cost of incremental evaluation is much cheaper than global evaluation* – It costs $\Theta(n)$ to evaluate the cost of an arbitrary n-vertex candidate TSP solution, because we must total the cost of each edge in the circular permutation describing the tour. Once that is found, however, the cost of the tour after swapping a given pair of vertices can be determined in constant time.

  If we are given a very large value of n and a very small budget of how much time we can spend searching, we are better off using it to do several incremental evaluations than a few random samples, even if we are looking for a needle in a haystack.

The primary drawback of a local search is that soon there isn't anything left for us to do as we find the local optimum. Sure, if we have more time we could start from different random points, but in landscapes of many low hills we are unlikely to stumble on the optimum.

How does local search do on TSP? Much better than random sampling for a similar amount of time. With over a total of 1.5 million tour evaluations in our 48-city TSP instance, our best local search tour had a length of 40,121.2—only 19.6% more than the optimal tour of 33,523.7.

This is good, but not great. You would not be happy to learn you are paying 19.6% more taxes than you should. Figure 7.9 illustrates the trajectory of a local search: repeated streaks from random tours down to decent solutions of fairly similar quality. We need more powerful methods to get closer to the optimal solution.

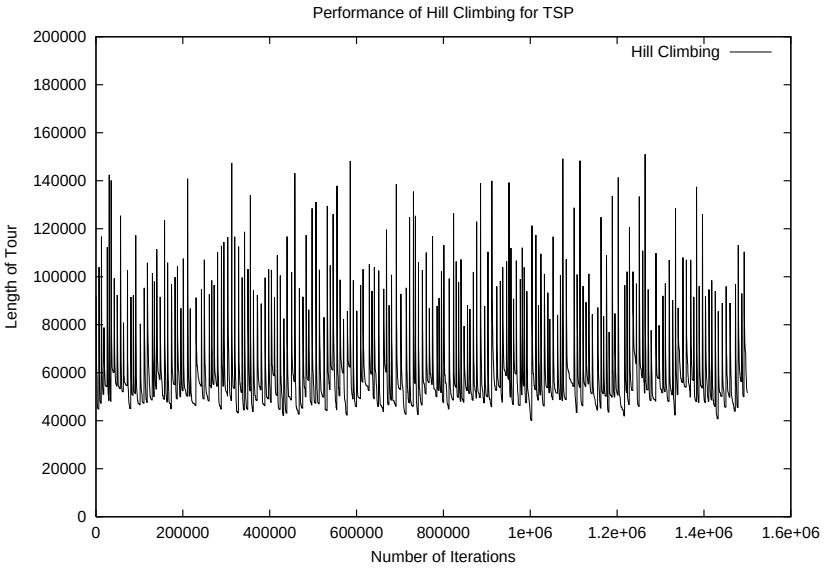

Figure 7.9: Search time/quality tradeoffs for TSP using hill climbing.

7.5.3 Simulated Annealing

Simulated annealing is a heuristic search procedure that allows occasional transitions leading to more expensive (and hence inferior) solutions. This may not sound like progress, but it helps keep our search from getting stuck in local optima. That poor fellow trapped on the top floor of a ski lodge would do better to break the glass and jump out the window if he really wanted to reach the top of the mountain.

The inspiration for simulated annealing comes from the physical process of cooling molten materials down to the solid state. In thermodynamic theory, the energy state of a system is described by the energy state of each particle constituting it. A particle's energy state jumps about randomly, with such transitions governed by the temperature of the system. In particular, the transition probability $P(e_i, e_j, T)$ from energy e_i to e_j at temperature T is given by

$$P(e_i, e_j, T) = e^{(e_i - e_j)/(k_B T)}$$

where k_B is a constant—called Boltzmann's constant.

What does this formula mean? Consider the value of the exponent under different conditions. The probability of moving from a high-energy state to a lower-energy state is very high. But, there is still a nonzero probability of accepting a

transition into a high-energy state, with such small jumps much more likely than big ones. The higher the temperature, the more likely energy jumps will occur.

```
Simulated-Annealing()
    Create initial solution S
    Initialize temperature t
    repeat
        for i = 1 to iteration-length do
            Generate a random transition from S to S_i
            If (C(S) ≥ C(S_i)) then S = S_i
            else if (e^((C(S)−C(S_i))/(k·t)) > random[0,1)) then S = S_i
        Reduce temperature t
    until (no change in C(S))
    Return S
```

What relevance does this have for combinatorial optimization? A physical system, as it cools, seeks to reach a minimum-energy state. Minimizing the total energy is a combinatorial optimization problem for any set of discrete particles. Through random transitions generated according to the given probability distribution, we can mimic the physics to solve arbitrary combinatorial optimization problems.

Take-Home Lesson: Forget about this molten metal business. Simulated annealing is effective because it spends much more of its time working on good elements of the solution space than on bad ones, and because it avoids getting trapped repeatedly in the same local optima.

As with a local search, the problem representation includes both a representation of the solution space and an easily computable cost function $C(s)$ measuring the quality of a given solution. The new component is the *cooling schedule*, whose parameters govern how likely we are to accept a bad transition as a function of time.

At the beginning of the search, we are eager to use randomness to explore the search space widely, so the probability of accepting a negative transition should be high. As the search progresses, we seek to limit transitions to local improvements and optimizations. The cooling schedule can be regulated by the following parameters:

- *Initial system temperature* – Typically $t_1 = 1$.
- *Temperature decrement function* – Typically $t_k = \alpha \cdot t_{k-1}$, where $0.8 \leq \alpha \leq 0.99$. This implies an exponential decay in the temperature, as opposed to a linear decay.
- *Number of iterations between temperature change* – Typically, 100 to 1,000 iterations might be permitted before lowering the temperature.

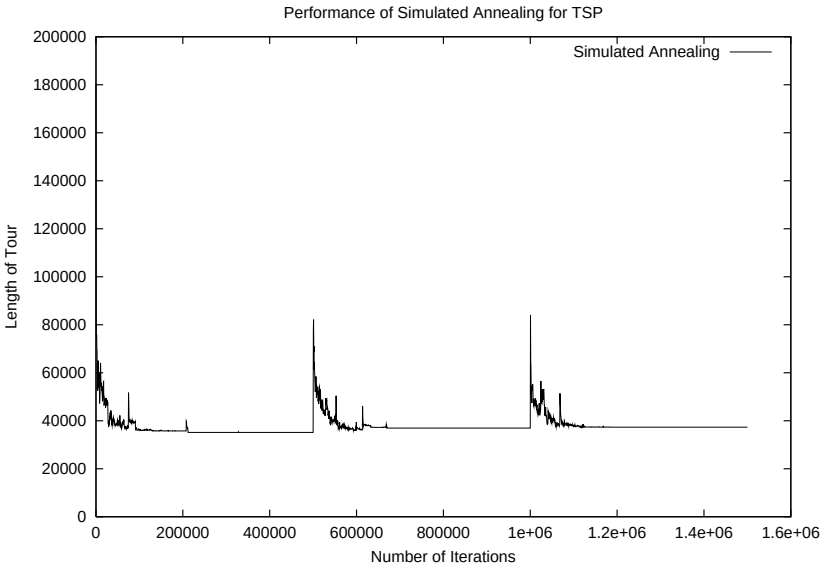

Figure 7.10: Search time/quality tradeoffs for TSP using simulated annealing

- *Acceptance criteria* – A typical criterion is to accept any transition from s_i to s_{i+1} when $C(s_{i+1}) < C(s_i)$, and also accept a negative transition whenever

  $$e^{-\frac{(C(s_i)-C(s_{i+1}))}{k \cdot t_i}} \geq r,$$

  where r is a random number $0 \leq r < 1$. The constant k normalizes this cost function so that almost all transitions are accepted at the starting temperature.

- *Stop criteria* – Typically, when the value of the current solution has not changed or improved within the last iteration or so, the search is terminated and the current solution reported.

Creating the proper cooling schedule is somewhat of a trial-and-error process of mucking with constants and seeing what happens. It probably pays to start from an existing implementation of simulated annealing, so check out my full implementation (at *http://www.algorist.com*) as well as others provided in Section 13.5 (page 407).

Compare the search/time execution profiles of our three heuristics. The cloud of points corresponding to random sampling is significantly worse than the solutions

encountered by the other heuristics. The scores of the short streaks corresponding to runs of hill-climbing solutions are clearly much better.

But best of all are the profiles of the three simulated annealing runs in Figure 7.10. All three runs lead to much better solutions than the best hill-climbing result. Further, it takes relatively few iterations to score most of the improvement, as shown by the three rapid plunges toward optimum we see with simulated annealing.

Using the same 1,500,000 iterations as the other methods, simulated annealing gave us a solution of cost 36,617.4—only 9.2% over the optimum. Even better solutions are available to those willing to wait a few minutes. Letting it run for 5,000,000 iterations got the score down to 34,254.9, or 2.2% over the optimum. There were no further improvements after I cranked it up to 10,000,000 iterations.

In expert hands, the best problem-specific heuristics for TSP can slightly outperform simulated annealing. But the simulated annealing solution works admirably. It is my heuristic method of choice.

Implementation

The implementation follows the pseudocode quite closely:

```
anneal(tsp_instance *t, tsp_solution *s)
{
  int i1, i2;                  /* pair of items to swap */
  int i,j;                     /* counters */
  double temperature;          /* the current system temp */
  double current_value;        /* value of current state */
  double start_value;          /* value at start of loop */
  double delta;                /* value after swap */
  double merit, flip;          /* hold swap accept conditions*/
  double exponent;             /* exponent for energy funct*/
  double random_float();
  double solution_cost(), transition();

  temperature = INITIAL_TEMPERATURE;

  initialize_solution(t->n,s);
  current_value = solution_cost(s,t);

  for (i=1; i<=COOLING_STEPS; i++) {
          temperature *= COOLING_FRACTION;

          start_value = current_value;

          for (j=1; j<=STEPS_PER_TEMP; j++) {
```

```
            /* pick indices of elements to swap */
            i1 = random_int(1,t->n);
            i2 = random_int(1,t->n);

            flip = random_float(0,1);

            delta = transition(s,t,i1,i2);
            exponent = (-delta/current_value)/(K*temperature);
            merit = pow(E,exponent);

            if (delta < 0)                              /*ACCEPT-WIN*/
                 current_value = current_value+delta;
            else { if (merit > flip)                    /*ACCEPT-LOSS*/
                 current_value = current_value+delta;
            else                                        /* REJECT */
                 transition(s,t,i1,i2);
            }
          }

          /* restore temperature if progress has been made */
          if ((current_value-start_value) < 0.0)
                 temperature = temperature/COOLING_FRACTION;
  }
}
```

7.5.4 Applications of Simulated Annealing

We provide several examples to demonstrate how these components can lead to elegant simulated annealing solutions for real combinatorial search problems.

Maximum Cut

The "maximum cut" problem seeks to partition the vertices of a weighted graph G into sets V_1 and V_2 to maximize the weight (or number) of edges with one vertex in each set. For graphs that specify an electronic circuit, the maximum cut in the graph defines the largest amount of data communication that can take place in the circuit simultaneously. As discussed in Section 16.6 (page 541), maximum cut is NP-complete.

How can we formulate maximum cut for simulated annealing? The solution space consists of all 2^{n-1} possible vertex partitions. We save a factor of two over all vertex subsets because vertex v_1 can be assumed to be fixed on the left side of the partition. The subset of vertices accompanying it can be represented using

a bit vector. The cost of a solution is the sum of the weights cut in the current configuration. A natural transition mechanism selects one vertex at random and moves it across the partition simply by flipping the corresponding bit in the bit vector. The change in the cost function will be the weight of its old neighbors minus the weight of its new neighbors. This can be computed in time proportional to the degree of the vertex.

This kind of simple, natural modeling is the right type of heuristic to seek in practice.

Independent Set

An "independent set" of a graph G is a subset of vertices S such that there is no edge with both endpoints in S. The maximum independent set of a graph is the largest such empty induced subgraph. Finding large independent sets arises in dispersion problems associated with facility location and coding theory, as discussed in Section 16.2 (page 528).

The natural state space for a simulated annealing solution would be all 2^n subsets of the vertices, represented as a bit vector. As with maximum cut, a simple transition mechanism would add or delete one vertex from S.

One natural cost function for subset S might be 0 if S contains an edge, and $|S|$ if it is indeed an independent set. This function ensures that we work towards an independent set at all times. However, this condition is strict enough that we are liable to move only in a narrow portion of the possible search space. More flexibility in the search space and quicker cost function computations can result from allowing nonempty graphs at the early stages of cooling. Better in practice would be a cost function like $C(S) = |S| - \lambda \cdot m_S/T$, where λ is a constant, T is the temperature, and m_S is the number of edges in the subgraph induced by S. The dependence of $C(S)$ on T ensures that the search will drive the edges out faster as the system cools.

Circuit Board Placement

In designing printed circuit boards, we are faced with the problem of positioning modules (typically, integrated circuits) on the board. Desired criteria in a layout may include (1) minimizing the area or aspect ratio of the board so that it properly fits within the allotted space, and (2) minimizing the total or longest wire length in connecting the components. Circuit board placement is representative of the kind of messy, multicriterion optimization problems for which simulated annealing is ideally suited.

Formally, we are given a collection of rectangular modules $r_1, \ldots, r_n$, each with associated dimensions $h_i \times l_i$. Further, for each pair of modules r_i, r_j, we are given the number of wires w_{ij} that must connect the two modules. We seek a placement of the rectangles that minimizes area and wire length, subject to the constraint that no two rectangles overlap each other.

The state space for this problem must describe the positions of each rectangle. To make this discrete, the rectangles can be restricted to lie on vertices of an integer grid. Reasonable transition mechanisms including moving one rectangle to a different location, or swapping the position of two rectangles. A natural cost function would be

$$C(S) = \lambda_{area}(S_{height} \cdot S_{width}) + \sum_{i=1}^{n}\sum_{j=1}^{n}(\lambda_{wire} \cdot w_{ij} \cdot d_{ij} + \lambda_{overlap}(r_i \cap r_j))$$

where λ_{area}, λ_{wire}, and $\lambda_{overlap}$ are constants governing the impact of these components on the cost function. Presumably, $\lambda_{overlap}$ should be an inverse function of temperature, so after gross placement it adjusts the rectangle positions to be disjointed.

Take-Home Lesson: Simulated annealing is a simple but effective technique for efficiently obtaining good but not optimal solutions to combinatorial search problems.

7.6 War Story: Only it is Not a Radio

"Think of it as a radio," he chuckled. "Only it is not a radio."

I'd been whisked by corporate jet to the research center of a large but very secretive company located somewhere east of California. They were so paranoid that I never got to see the object we were working on, but the people who brought me in did a great job of abstracting the problem.

The application concerned a manufacturing technique known as *selective assembly*. Eli Whitney started the Industrial Revolution through his system of *interchangeable parts*. He carefully specified the manufacturing tolerances on each part in his machine so that the parts were *interchangeable*, meaning that any legal cog-widget could be used to replace any other legal cog-widget. This greatly sped up the process of manufacturing, because the workers could just put parts together instead of having to stop to file down rough edges and the like. It made replacing broken parts a snap. This was a very good thing.

Unfortunately, it also resulted in large piles of cog-widgets that were slightly outside the manufacturing tolerance and thus had to be discarded. Another clever fellow then observed that maybe one of these defective cog-widgets could be used when all the *other* parts in the given assembly *exceeded* their required manufacturing tolerances. Good plus bad could well equal good enough. This is the idea of *selective assembly*.

"Each not-radio is made up of n different types of not-radio parts," he told me. For the ith part type (say the right flange gasket), we have a pile of s_i instances of this part type. Each part (flange gasket) comes with a measure of the degree to which it deviates from perfection. We need to match up the parts so as to create the greatest number of working not-radios as possible."

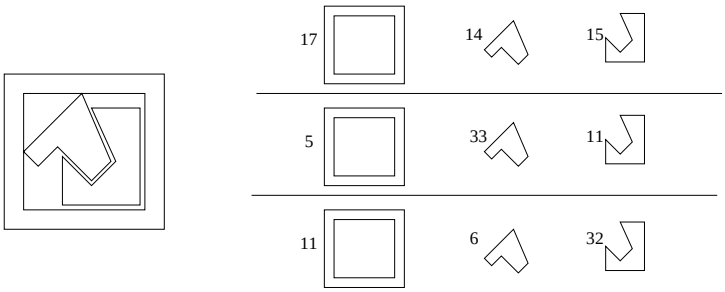

Figure 7.11: Part assignments for three not-radios, such that each had at most 50 points total defect

The situation is illustrated in Figure 7.11. Each not-radio consists of three parts, and the sum of the defects in any functional not-radio must total at most 50. By cleverly balancing the good and bad parts in each machine, we can use all the parts and make three working not-radios.

I thought about the problem. The simplest procedure would take the best part for each part type, make a not-radio out of them, and repeat until the not-radio didn't play (or do whatever a not-radio does). But this would create a small number of not-radios drastically varying in quality, whereas they wanted as many decent not-radios as possible.

The goal was to match up good parts and bad parts so the total amount of badness wasn't so bad. Indeed, the problem sounded related to *matching* in graphs (see Section 15.6 (page 498)). Suppose we built a graph where the vertices were the part instances, and add an edge for all two part instances that were within the total error tolerance. In graph matching, we seek the largest number of edges such that no vertex appears more than once in the matching. This is analogous to the largest number of two-part assemblies we can form from the given set of parts.

"I can solve your problem using matching," I announced, "Provided not-radios are each made of only two parts."

There was silence. Then they all started laughing at me. "*Everyone* knows not-radios have more than two parts," they said, shaking their heads.

That spelled the end of this algorithmic approach. Extending to more than two parts turned the problem into matching on hypergraphs,[2]—a problem which is NP-complete. Further, it might take exponential time in the number of part types just to build the graph, since we had to explicitly construct each possible hyperedge/assembly.

[2]A *hypergraph* is made up of edges that can contain more than two vertices each. They can be thought of as general collections of subsets of vertices/elements.

I went back to the drawing board. They wanted to put parts into assemblies so that no assembly would have more total defects than allowed. Described that way, it sounded like a packing problem. In the *bin packing* problem (see Section 17.9 (page 595)), we are given a collection of items of different sizes and asked to store them using the smallest possible number of bins, each of which has a fixed capacity of size k. Here, the assemblies represented the bins, each of which could absorb total defect $\leq k$. The items to pack represented the individual parts, whose size would reflect its quality of manufacture.

It wasn't pure bin packing, however, since parts came in different types. The application imposed constraints on the allowable contents of each bin. Creating the maximum number of not-radios meant that we sought a packing that maximized the number of bins which contained exactly one part for each of the m different parts types.

Bin packing is NP-complete, but is a natural candidate for a heuristic search approach. The solution space consists of assignments of parts to bins. We initially pick a random part of each type for each bin to give us a starting configuration for the search.

The local neighborhood operation involves moving parts around from one bin to another. We could move one part at a time, but more effective was *swapping* parts of a particular type between two randomly chosen bins. In such a swap, both bins remain complete not-radios, hopefully with better error tolerance than before. Thus, our swap operator required three random integers—one to select the appropriate parts type (from 1 to m) and two more to select the assembly bins involved (say from 1 to b).

The key decision was the cost function to use. They supplied the hard limit k on the total defect level for each *individual* assembly. But what was the best way to score a *set* of assemblies? We could just return the number of acceptable complete assemblies as our score—an integer from 1 to b. Although this was indeed what we wanted to optimize, it would not be sensitive to detect when we were making partial progress towards a solution. Suppose one of our swaps succeeded in bringing one of the nonfunctional assemblies much closer to the not-radio limit k. That would be a better starting point for further progress than the original, and should be favored.

My final cost function was as follows. I gave one point for every working assembly, and a significantly smaller total for each nonworking assembly based on how close it was to the threshold k. The score for a nonworking assembly decreased exponentially based on how much it was over k. Thus the optimizer would seek to maximize the number of working assemblies, and then try to drive another assembly close to the limit.

I implemented this algorithm, and then ran the search on the test case they provided. It was an instance taken directly from the factory floor. Not-radios turn out to contain $m = 8$ important parts types. Some parts types are more expensive than others, and so they have fewer available candidates to consider. The most

	suffix			
prefix	AA	AG	GA	GG
AA	$AAAA$	$AAAG$	$AAGA$	$AAGG$
AG	$AGAA$	$AGAG$	$AGGA$	$AGGG$
GA	$GAAG$	$GAAG$	$GAGA$	$GAGG$
GG	$GGAA$	$GGAG$	$GGGA$	$GGGG$

Figure 7.12: A prefix-suffix array of all purine 4-mers

constrained parts type had only eight representatives, so there could be at most eight possible assemblies from this given mix.

I watched as simulated annealing chugged and bubbled on the problem instance. The number of completed assemblies instantly climbed (1, 2, 3, 4) before progress started to slow a bit. Then came 5 and 6 in a hiccup, with a pause before assembly 7 came triumphantly together. But tried as it might, the program could not put together eight not-radios before I lost interest in watching.

I called and tried to admit defeat, but they wouldn't hear it. It turns out that the best the factory had managed after extensive efforts was only *six* working not-radios, so my result represented a significant improvement!

7.7 War Story: Annealing Arrays

The war story of Section 3.9 (page 94) reported how we used advanced data structures to simulate a new method for sequencing DNA. Our method, interactive sequencing by hybridization (SBH), required building arrays of specific oligonucleotides on demand.

A biochemist at Oxford University got interested in our technique, and moreover he had in his laboratory the equipment we needed to test it out. The Southern Array Maker, manufactured by Beckman Instruments, prepared discrete oligonucleotide sequences in 64 parallel rows across a polypropylene substrate. The device constructs arrays by appending single characters to each cell along specific rows and columns of arrays. Figure 7.12 shows how to construct an array of all $2^4 = 16$ purine (A or G) 4-mers by building the prefixes along rows and the suffixes along columns. This technology provided an ideal environment for testing the feasibility of interactive SBH in a laboratory, because with proper programming it gave a way to fabricate a wide variety of oligonucleotide arrays on demand.

However, we had to provide the proper programming. Fabricating complicated arrays required solving a difficult combinatorial problem. We were given as input a set of n strings (representing oligonucleotides) to fabricate in an $m \times m$ array (where $m = 64$ on the Southern apparatus). We had to produce a schedule of row and column commands to realize the set of strings S. We proved that the

problem of designing dense arrays was NP-complete, but that didn't really matter. My student Ricky Bradley and I had to solve it anyway.

"We are going to have to use a heuristic," I told him. "So how can we model this problem?"

"Well, each string can be partitioned into prefix and suffix pairs that realize it. For example, the string ACC can be realized in four different ways: prefix '' and suffix ACC, prefix A and suffix CC, prefix AC and suffix C, or prefix ACC and suffix ''. We seek the smallest set of prefixes and suffixes that together realize all the given strings," Ricky said.

"Good. This gives us a natural representation for simulated annealing. The state space will consist of all possible subsets of prefixes and suffixes. The natural transitions between states might include inserting or deleting strings from our subsets, or swapping a pair in or out."

"What's a good cost function?" he asked.

"Well, we need as small an array as possible that covers all the strings. How about taking the maximum of number of rows (prefixes) or columns (suffixes) used in our array, plus the number of strings from S that are not yet covered. Try it and let's see what happens."

Ricky went off and implemented a simulated annealing program along these lines. It printed out the state of the solution each time a transition was accepted and was fun to watch. The program quickly kicked out unnecessary prefixes and suffixes, and the array began shrinking rapidly in size. But after several hundred iterations, progress started to slow. A transition would knock out an unnecessary suffix, wait a while, then add a different suffix back again. After a few thousand iterations, no real improvement was happening.

"The program doesn't seem to recognize when it is making progress. The evaluation function only gives credit for minimizing the larger of the two dimensions. Why not add a term to give some credit to the other dimension."

Ricky changed the evaluation function, and we tried again. This time, the program did not hesitate to improve the shorter dimension. Indeed, our arrays started to be skinny rectangles instead of squares.

"OK. Let's add another term to the evaluation function to give it points for being roughly square."

Ricky tried again. Now the arrays were the right shape, and progress was in the right direction. But the progress was still slow.

"Too many of the insertion moves don't affect many strings. Maybe we should skew the random selections so that the important prefix/suffixes get picked more often."

Ricky tried again. Now it converged faster, but sometimes it still got stuck. We changed the cooling schedule. It did better, but was it doing well? Without a lower bound knowing how close we were to optimal, it couldn't really tell how good our solution was. We tweaked and tweaked until our program stopped improving.

Our final solution refined the initial array by applying the following random moves:

Figure 7.13: Compression of the HIV array by simulated annealing – after 0, 500, 1,000, and 5,750 iterations

---

- *swap* – swap a prefix/suffix on the array with one that isn't.
- *add* – add a random prefix/suffix to the array.
- *delete* – delete a random prefix/suffix from the array.
- *useful add* – add the prefix/suffix with the highest usefulness to the array.
- *useful delete* – delete the prefix/suffix with the lowest usefulness from the array.
- *string add* – randomly select a string not on the array, and add the most useful prefix and/or suffix to cover this string.

A standard cooling schedule was used, with an exponentially decreasing temperature (dependent upon the problem size) and a temperature-dependent Boltzmann criterion for accepting states that have higher costs. Our final cost function was defined as

$$cost = 2 \times max + min + \frac{(max - min)^2}{4} + 4(str_{total} - str_{in})$$

where max is the size of the maximum chip dimension, min is the size of the minimum chip dimension, $str_{total} = |S|$, and str_{in} is the number of strings from S currently on the chip.

How well did we do? Figure 7.13 shows the convergence of a custom array consisting of the 5,716 unique 7-mers of the HIV virus. Figure 7.13 shows snapshots of the state of the chip at four points during the annealing process (0, 500, 1,000, and the final chip at 5,750 iterations). Black pixels represent the first occurrence of an HIV 7-mer. The final chip size here is 130×132—quite an improvement over

the initial size of 192×192. It took about fifteen minutes' worth of computation to complete the optimization, which was perfectly acceptable for the application.

But how well did we do? Since simulated annealing is only a heuristic, we really don't know how close to optimal our solution is. I think we did pretty well, but can't really be sure. Simulated annealing is a good way to handle complex optimization problems. However, to get the best results, expect to spend more time tweaking and refining your program than you did in writing it in the first place. This is dirty work, but sometimes you have to do it.

7.8 Other Heuristic Search Methods

Several heuristic search methods have been proposed to search for good solutions for combinatorial optimization problems. Like simulated annealing, many techniques relies on analogies to real-world physical processes. Popular methods include *genetic algorithms*, *neural networks*, and *ant colony optimization*.

The intuition behind these methods is highly appealing, but skeptics decry them as voodoo optimization techniques that rely more on nice analogies to nature than demonstrated computational results on problems that have been studied using other methods.

The question isn't whether you can get decent answers for many problems given enough effort using these techniques. Clearly you can. The real question is whether they lead to *better* solutions with *less implementation complexity* than the other methods we have discussed.

In general, I don't believe that they do. But in the spirit of free inquiry, I introduce genetic algorithms, which is the most popular of these methods. See the chapter notes for more detailed readings.

Genetic Algorithms

Genetic algorithms draw their inspiration from evolution and natural selection. Through the process of natural selection, organisms adapt to optimize their chances for survival in a given environment. Random mutations occur in an organism's genetic description, which then get passed on to its children. Should a mutation prove helpful, these children are more likely to survive and reproduce. Should it be harmful, these children won't, and so the bad trait will die with them.

Genetic algorithms maintain a "population" of solution candidates for the given problem. Elements are drawn at random from this population and allowed to "reproduce" by combining aspects of the two-parent solutions. The probability that an element is chosen to reproduce is based on its "fitness,"—essentially the cost of the solution it represents. Unfit elements die from the population, to be replaced by a successful-solution offspring.

The idea behind genetic algorithms is extremely appealing. However, they don't seem to work as well on practical combinatorial optimization problems as simulated

annealing does. There are two primary reasons for this. First, it is quite unnatural to model applications in terms of genetic operators like mutation and crossover on bit strings. The pseudobiology adds another level of complexity between you and your problem. Second, genetic algorithms take a very long time on nontrivial problems. The crossover and mutation operations typically make no use of problem-specific structure, so most transitions lead to inferior solutions, and convergence is slow. Indeed, the analogy with evolution—where significant progress require millions of years—can be quite appropriate.

We will not discuss genetic algorithms further, to discourage you from considering them for your applications. However, pointers to implementations of genetic algorithms are provided in Section 13.5 (page 407) if you really insist on playing with them.

> *Take-Home Lesson:* I have *never* encountered any problem where genetic algorithms seemed to me the right way to attack it. Further, I have *never* seen any computational results reported using genetic algorithms that have favorably impressed me. Stick to simulated annealing for your heuristic search voodoo needs.

7.9 Parallel Algorithms

Two heads are better than one, and more generally, n heads are better than $n-1$. Parallel processing is becoming more important with the advent of cluster computing and multicore processors. It seems like the easy way out of hard problems. Indeed, sometimes, for some problems, parallel algorithms are the most effective solution. High-resolution, real-time graphics applications must render thirty frames per second for realistic animation. Assigning each frame to a distinct processor, or dividing each image into regions assigned to different processors, might be the only way to get the job done in time. Large systems of linear equations for scientific applications are routinely solved in parallel.

However, there are several pitfalls associated with parallel algorithms that you should be aware of:

- *There is often a small upper bound on the potential win* – Suppose that you have access to twenty processors that can be devoted exclusively to your job. Potentially, these could be used to speed up the fastest sequential program by up to a factor of twenty. That is nice, but greater performance gains maybe possible by finding a better sequential algorithm. Your time spent parallelizing a code might well be better spent enhancing the sequential version. Performance-tuning tools such as profilers are better developed for sequential machines than for parallel models.

- *Speedup means nothing* – Suppose my parallel program runs 20 times faster on a 20-processor machine than it does on one processor. That's great, isn't

it? If you always get linear speedup and have an arbitrary number of processors, you will eventually beat any sequential algorithm. However, a carefully designed sequential algorithm can often beat an easily-parallelized code running on a typical parallel machine. The one-processor parallel version of your code is likely to be a crummy sequential algorithm, so measuring speedup typically provides an unfair test of the benefits of parallelism.

The classic example of this occurs in the minimax game-tree search algorithm used in computer chess programs. A brute-force tree search is embarrassingly easy to parallelize: just put each subtree on a different processor. However, a lot of work gets wasted because the same positions get considered on different machines. Moving from a brute-force search to the more clever alpha-beta pruning algorithm can easily save 99.99% of the work, thus dwarfing any benefits of a parallel brute-force search. Alpha-beta can be parallelized, but not easily, and the speedups grow surprisingly slowly as a function of the number of processors you have.

- *Parallel algorithms are tough to debug* – Unless your problem can be decomposed into several independent jobs, the different processors must communicate with each other to end up with the correct final result. Unfortunately, the nondeterministic nature of this communication makes parallel programs notoriously difficult to debug. Perhaps the best example is *Deep Blue*—the world-champion chess computer. Although it eventually beat Kasparov, over the years it lost several games in embarrassing fashion due to bugs, mostly associated with its extensive parallelism.

I recommend considering parallel processing only after attempts at solving a problem sequentially prove too slow. Even then, I would restrict attention to algorithms that parallelize the problem by partitioning the input into distinct tasks where no communication is needed between the processors, except to collect the final results. Such large-grain, naive parallelism can be simple enough to be both implementable and debuggable, because it really reduces to producing a good sequential implementation. There can be pitfalls even in this approach, however, as shown in the war story below.

7.10 War Story: Going Nowhere Fast

In Section 2.8 (page 51), I related our efforts to build a fast program to test Waring's conjecture for pyramidal numbers. At that point, my code was fast enough that it could complete the job in a few weeks running in the background of a desktop workstation. This option did not appeal to my supercomputing colleague, however.

"Why don't we do it in parallel?" he suggested. "After all, you have an outer loop doing the same calculation on each integer from 1 to 1,000,000,000. I can split this range of numbers into different intervals and run each range on a different processor. Watch, it will be easy."

He set to work trying to do our computations on an Intel IPSC-860 hypercube using 32 nodes with 16 megabytes of memory per node—very big iron for the time. However, instead of getting answers, I was treated to a regular stream of e-mail about system reliability over the next few weeks:

- "Our code is running fine, except one processor died last night. I will rerun."
- "This time the machine was rebooted by accident, so our long-standing job was killed."
- "We have another problem. The policy on using our machine is that nobody can command the entire machine for more than thirteen hours, under any condition."

Still, eventually, he rose to the challenge. Waiting until the machine was stable, he locked out 16 processors (half the computer), divided the integers from 1 to 1,000,000,000 into 16 equal-sized intervals, and ran each interval on its own processor. He spent the next day fending off angry users who couldn't get their work done because of our rogue job. The instant the first processor completed analyzing the numbers from 1 to 62,500,000, he announced to all the people yelling at him that the rest of the processors would soon follow.

But they didn't. He failed to realize that the time to test each integer increased as the numbers got larger. After all, it would take longer to test whether 1,000,000,000 could be expressed as the sum of three pyramidal numbers than it would for 100. Thus, at slower and slower intervals each new processor would announce its completion. Because of the architecture of the hypercube, he couldn't return any of the processors until our entire job was completed. Eventually, half the machine and most of its users were held hostage by one, final interval.

What conclusions can be drawn from this? If you are going to parallelize a problem, be sure to balance the load carefully among the processors. Proper load balancing, using either back-of-the-envelope calculations or the partition algorithm we will develop in Section 8.5 (page 294), would have significantly reduced the time we needed the machine, and his exposure to the wrath of his colleagues.

Chapter Notes

The treatment of backtracking here is partially based on my book *Programming Challenges* [SR03]. In particular, the `backtrack` routine presented here is a generalization of the version in Chapter 8 of [SR03]. Look there for my solution to the famous *eight queens problem*, which seeks all chessboard configurations of eight mutually nonattacking queens on an 8×8 board.

The original paper on simulated annealing [KGV83] included an application to VLSI module placement problems. The applications from Section 7.5.4 (page 258) are based on material from [AK89].

The heuristic TSP solutions presented here employ vertex-swap as the local neighborhood operation. In fact, edge-swap is a more powerful operation. Each edge-swap changes two edges in the tour at most, as opposed to at most four edges with a vertex-swap. This improves the possibility of a local improvement. However, more sophisticated data structures are necessary to efficiently maintain the order of the resulting tour [FJMO93].

The different heuristic search techniques are ably presented in Aarts and Lenstra [AL97], which I strongly recommend for those interested in learning more about heuristic searches. Their coverage includes *tabu search*, a variant of simulated annealing that uses extra data structures to avoid transitions to recently visited states. Ant colony optimization is discussed in [DT04]. See [MF00] for a more favorable view of genetic algorithms and the like.

More details on our combinatorial search for optimal chessboard-covering positions appear in our paper [RHS89]. Our work using simulated annealing to compress DNA arrays was reported in [BS97]. See Pugh [Pug86] and Coullard et al. [CGJ98] for more on selective assembly. Our parallel computations on pyramidal numbers were reported in [DY94].

7.11 Exercises

Backtracking

7-1. *[3]* A *derangement* is a permutation p of $\{1, \ldots, n\}$ such that no item is in its proper position, i.e. $p_i \neq i$ for all $1 \leq i \leq n$. Write an efficient backtracking program with pruning that constructs all the derangements of n items.

7-2. *[4] Multisets* are allowed to have repeated elements. A multiset of n items may thus have fewer than $n!$ distinct permutations. For example, $\{1, 1, 2, 2\}$ has only six different permutations: $\{1, 1, 2, 2\}$, $\{1, 2, 1, 2\}$, $\{1, 2, 2, 1\}$, $\{2, 1, 1, 2\}$, $\{2, 1, 2, 1\}$, and $\{2, 2, 1, 1\}$. Design and implement an efficient algorithm for constructing all permutations of a multiset.

7-3. *[5]* Design and implement an algorithm for testing whether two graphs are isomorphic to each other. The graph isomorphism problem is discussed in Section 16.9 (page 550). With proper pruning, graphs on hundreds of vertices can be tested reliably.

7-4. *[5]* Anagrams are rearrangements of the letters of a word or phrase into a different word or phrase. Sometimes the results are quite striking. For example, "MANY VOTED BUSH RETIRED" is an anagram of "TUESDAY NOVEMBER THIRD," which correctly predicted the result of the 1992 U.S. presidential election. Design and implement an algorithm for finding anagrams using combinatorial search and a dictionary.

7-5. *[8]* Design and implement an algorithm for solving the subgraph isomorphism problem. Given graphs G and H, does there exist a subgraph H' of H such that G is isomorphic to H'? How does your program perform on such special cases of subgraph isomorphism as Hamiltonian cycle, clique, independent set, and graph isomorphism?

7-6. *[8]* In the turnpike reconstruction problem, you are given $n(n-1)/2$ distances in sorted order. The problem is to find the positions of n points on the line that give rise to these distances. For example, the distances $\{1, 2, 3, 4, 5, 6\}$ can be determined by placing the second point 1 unit from the first, the third point 3 from the second, and the fourth point 2 from the third. Design and implement an efficient algorithm to report all solutions to the turnpike reconstruction problem. Exploit additive constraints when possible to minimize the search. With proper pruning, problems with hundreds of points can be solved reliably.

Combinatorial Optimization

For each of the problems below, either (1) implement a combinatorial search program to solve it optimally for small instance, and/or (2) design and implement a simulated annealing heuristic to get reasonable solutions. How well does your program perform in practice?

7-7. *[5]* Design and implement an algorithm for solving the bandwidth minimization problem discussed in Section 13.2 (page 398).

7-8. *[5]* Design and implement an algorithm for solving the maximum satisfiability problem discussed in Section 14.10 (page 472).

7-9. *[5]* Design and implement an algorithm for solving the maximum clique problem discussed in Section 16.1 (page 525).

7-10. *[5]* Design and implement an algorithm for solving the minimum vertex coloring problem discussed in Section 16.7 (page 544).

7-11. *[5]* Design and implement an algorithm for solving the minimum edge coloring problem discussed in Section 16.8 (page 548).

7-12. *[5]* Design and implement an algorithm for solving the minimum feedback vertex set problem discussed in Section 16.11 (page 559).

7-13. *[5]* Design and implement an algorithm for solving the set cover problem discussed in Section 18.1 (page 621).

Interview Problems

7-14. *[4]* Write a function to find all permutations of the letters in a particular string.

7-15. *[4]* Implement an efficient algorithm for listing all k-element subsets of n items.

7-16. *[5]* An anagram is a rearrangement of the letters in a given string into a sequence of dictionary words, like *Steven Skiena* into *Vainest Knees*. Propose an algorithm to construct all the anagrams of a given string.

7-17. *[5]* Telephone keypads have letters on each numerical key. Write a program that generates all possible words resulting from translating a given digit sequence (e.g., 145345) into letters.

7-18. *[7]* You start with an empty room and a group of n people waiting outside. At each step, you may either admit one person into the room, or let one out. Can you arrange a sequence of 2^n steps, so that every possible combination of people is achieved exactly once?

7-19. *[4]* Use a random number generator (rng04) that generates numbers from $\{0, 1, 2, 3, 4\}$ with equal probability to write a random number generator that generates numbers from 0 to 7 (rng07) with equal probability. What are expected number of calls to rng04 per call of rng07?

Programming Challenges

These programming challenge problems with robot judging are available at *http://www.programming-challenges.com* or *http://online-judge.uva.es*.

7-1. "Little Bishops" – Programming Challenges 110801, UVA Judge 861.

7-2. "15-Puzzle Problem" – Programming Challenges 110802, UVA Judge 10181.

7-3. "Tug of War" – Programming Challenges 110805, UVA Judge 10032.

7-4. "Color Hash" – Programming Challenges 110807, UVA Judge 704.

8

Dynamic Programming

The most challenging algorithmic problems involve optimization, where we seek to find a solution that maximizes or minimizes some function. Traveling salesman is a classic optimization problem, where we seek the tour visiting all vertices of a graph at minimum total cost. But as shown in Chapter 1, it is easy to propose "algorithms" solving TSP that generate reasonable-looking solutions but did not *always* produce the minimum cost tour.

Algorithms for optimization problems require proof that they always return the best possible solution. Greedy algorithms that make the best local decision at each step are typically efficient but usually do not guarantee global optimality. Exhaustive search algorithms that try all possibilities and select the best always produce the optimum result, but usually at a prohibitive cost in terms of time complexity.

Dynamic programming combines the best of both worlds. It gives us a way to design custom algorithms that systematically search all possibilities (thus guaranteeing correctness) while storing results to avoid recomputing (thus providing efficiency). By storing the *consequences* of all possible decisions and using this information in a systematic way, the total amount of work is minimized.

Once you understand it, dynamic programming is probably the easiest algorithm design technique to apply in practice. In fact, I find that dynamic programming algorithms are often easier to reinvent than to try to look up in a book. That said, *until* you understand dynamic programming, it seems like magic. You must figure out the trick before you can use it.

Dynamic programming is a technique for efficiently implementing a recursive algorithm by storing partial results. The trick is seeing whether the naive recursive algorithm computes the same subproblems over and over and over again. If so, storing the answer for each subproblems in a table to look up instead of recompute

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can lead to an efficient algorithm. Start with a recursive algorithm or definition. Only once we have a correct recursive algorithm do we worry about speeding it up by using a results matrix.

Dynamic programming is generally the right method for optimization problems on combinatorial objects that have an inherent *left to right* order among components. Left-to-right objects includes: character strings, rooted trees, polygons, and integer sequences. Dynamic programming is best learned by carefully studying examples until things start to click. We present three war stories where dynamic programming played the decisive role to demonstrate its utility in practice.

8.1 Caching vs. Computation

Dynamic programming is essentially a tradeoff of space for time. Repeatedly recomputing a given quantity is harmless unless the time spent doing so becomes a drag on performance. Then we are better off storing the results of the initial computation and looking them up instead of recomputing them again.

The tradeoff between space and time exploited in dynamic programming is best illustrated when evaluating recurrence relations such as the Fibonacci numbers. We look at three different programs for computing them below.

8.1.1 Fibonacci Numbers by Recursion

The Fibonacci numbers were originally defined by the Italian mathematician Fibonacci in the thirteenth century to model the growth of rabbit populations. Rabbits breed, well, like rabbits. Fibonacci surmised that the number of pairs of rabbits born in a given year is equal to the number of pairs of rabbits born in each of the two previous years, starting from one pair of rabbits in the first year. To count the number of rabbits born in the nth year, he defined the recurrence relation:

$$F_n = F_{n-1} + F_{n-2}$$

with basis cases $F_0 = 0$ and $F_1 = 1$. Thus, $F_2 = 1$, $F_3 = 2$, and the series continues $\{3, 5, 8, 13, 21, 34, 55, 89, 144, \ldots\}$. As it turns out, Fibonacci's formula didn't do a very good job of counting rabbits, but it does have a host of interesting properties.

Since they are defined by a recursive formula, it is easy to write a recursive program to compute the nth Fibonacci number. A recursive function algorithm written in C looks like this:

```
long fib_r(int n)
{
        if (n == 0) return(0);
        if (n == 1) return(1);

        return(fib_r(n-1) + fib_r(n-2));
}
```

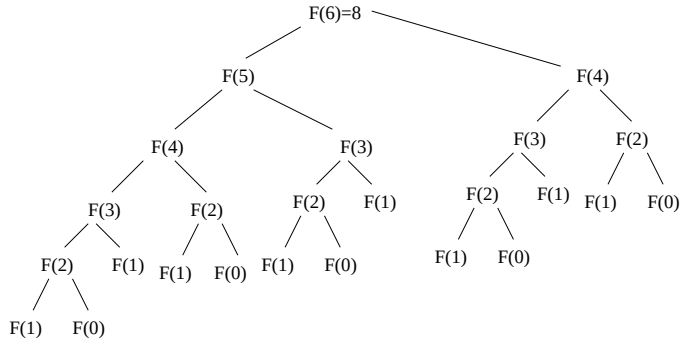

Figure 8.1: The computation tree for computing Fibonacci numbers recursively

The course of execution for this recursive algorithm is illustrated by its *recursion tree*, as illustrated in Figure 8.1. This tree is evaluated in a depth-first fashion, as are all recursive algorithms. I encourage you to trace this example by hand to refresh your knowledge of recursion.

Note that $F(4)$ is computed on both sides of the recursion tree, and $F(2)$ is computed no less than five times in this small example. The weight of all this redundancy becomes clear when you run the program. It took more than 7 minutes for my program to compute the first 45 Fibonacci numbers. You could probably do it faster by hand using the right algorithm.

How much time does this algorithm take to compute $F(n)$? Since $F_{n+1}/F_n \approx \phi = (1+\sqrt{5})/2 \approx 1.61803$, this means that $F_n > 1.6^n$. Since our recursion tree has only 0 and 1 as leaves, summing up to such a large number means we must have at least 1.6^n leaves or procedure calls! This humble little program takes exponential time to run!

8.1.2 Fibonacci Numbers by Caching

In fact, we can do much better. We can explicitly store (or *cache*) the results of each Fibonacci computation $F(k)$ in a table data structure indexed by the parameter k. The key to avoiding recomputation is to explicitly check for the value before trying to compute it:

```
#define MAXN    45       /* largest interesting n */
#define UNKNOWN   -1     /* contents denote an empty cell */
long f[MAXN+1];          /* array for caching computed fib values */
```

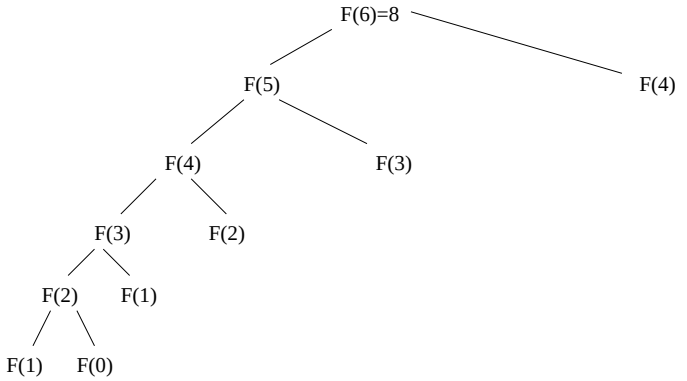

Figure 8.2: The Fibonacci computation tree when caching values

```
long fib_c(int n)
{
        if (f[n] == UNKNOWN)
                f[n] = fib_c(n-1) + fib_c(n-2);

        return(f[n]);
}


long fib_c_driver(int n)
{
        int i;                  /* counter */

        f[0] = 0;
        f[1] = 1;
        for (i=2; i<=n; i++)  f[i] = UNKNOWN;

        return(fib_c(n));
}
```

To compute $F(n)$, we call `fib_c_driver(n)`. This initializes our cache to the two values we initially know ($F(0)$ and $F(1)$) as well as the `UNKNOWN` flag for all the rest we don't. It then calls a look-before-crossing-the-street version of the recursive algorithm.

This cached version runs instantly up to the largest value that can fit in a long integer. The new recursion tree (Figure 8.2) explains why. There is no meaningful branching, because only the left-side calls do computation. The right-side calls find what they are looking for in the cache and immediately return.

What is the running time of this algorithm? The recursion tree provides more of a clue than the code. In fact, it computes $F(n)$ in linear time (in other words, $O(n)$ time) because the recursive function `fib_c(k)` is called exactly twice for each value $0 \leq k \leq n$.

This general method of explicitly caching results from recursive calls to avoid recomputation provides a simple way to get *most* of the benefits of full dynamic programming, so it is worth a more careful look. In principle, such caching can be employed on any recursive algorithm. However, storing partial results would have done absolutely no good for such recursive algorithms as *quicksort*, *backtracking*, and *depth-first search* because all the recursive calls made in these algorithms have distinct *parameter values*. It doesn't pay to store something you will never refer to again.

Caching makes sense only when the space of distinct parameter values is modest enough that we can afford the cost of storage. Since the argument to the recursive function `fib_c(k)` is an integer between 0 and n, there are only $O(n)$ values to cache. A linear amount of space for an exponential amount of time is an excellent tradeoff. But as we shall see, we can do even better by eliminating the recursion completely.

> *Take-Home Lesson:* Explicit caching of the results of recursive calls provides *most* of the benefits of dynamic programming, including usually the same running time as the more elegant full solution. If you prefer doing extra programming to more subtle thinking, you can stop here.

8.1.3 Fibonacci Numbers by Dynamic Programming

We can calculate F_n in linear time more easily by explicitly specifying the order of evaluation of the recurrence relation:

```
long fib_dp(int n)
{
        int i;              /* counter */
        long f[MAXN+1];     /* array to cache computed fib values */

        f[0] = 0;
        f[1] = 1;
        for (i=2; i<=n; i++)  f[i] = f[i-1]+f[i-2];

        return(f[n]);
}
```

We have removed all recursive calls! We evaluate the Fibonacci numbers from smallest to biggest and store all the results, so we know that we have F_{i-1} and F_{i-2} ready whenever we need to compute F_i. The linearity of this algorithm should

be apparent. Each of the n values is computed as the simple sum of two integers in total $O(n)$ time and space.

More careful study shows that we do not need to store all the intermediate values for the entire period of execution. Because the recurrence depends on two arguments, we only need to retain the last two values we have seen:

```
long fib_ultimate(int n)
{
        int i;                  /* counter */
        long back2=0, back1=1;  /* last two values of f[n] */
        long next;              /* placeholder for sum */

        if (n == 0) return (0);

        for (i=2; i<n; i++) {
                next = back1+back2;
                back2 = back1;
                back1 = next;
        }
        return(back1+back2);
}
```

This analysis reduces the storage demands to constant space with no asymptotic degradation in running time.

8.1.4 Binomial Coefficients

We now show how to compute the *binomial coefficients* as another illustration of how to eliminate recursion by specifying the order of evaluation. The binomial coefficients are the most important class of counting numbers, where $\binom{n}{k}$ counts the number of ways to choose k things out of n possibilities.

How do you compute the binomial coefficients? First, $\binom{n}{k} = n!/((n-k)!k!)$, so in principle you can compute them straight from factorials. However, this method has a serious drawback. Intermediate calculations can easily cause arithmetic overflow, even when the final coefficient fits comfortably within an integer.

A more stable way to compute binomial coefficients is using the recurrence relation implicit in the construction of Pascal's triangle:

```
                1
              1   1
            1   2   1
          1   3   3   1
        1   4   6   4   1
      1   5  10  10   5   1
```

m / n	0	1	2	3	4	5
0	A					
1	B	G				
2	C	1	H			
3	D	2	3	I		
4	E	4	5	6	J	
5	F	7	8	9	10	K

m / n	0	1	2	3	4	5
0	1					
1	1	1				
2	1	1	1			
3	1	3	3	1		
4	1	4	6	4	1	
5	1	5	10	10	**5**	1

Figure 8.3: Evaluation order for `binomial_coefficient` at $M[5,4]$ (l). Initialization conditions A-K, recurrence evaluations 1-10. Matrix contents after evaluation (r)

Each number is the sum of the two numbers directly above it. The recurrence relation implicit in this is that

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

Why does this work? Consider whether the nth element appears in one of the $\binom{n}{k}$ subsets of k elements. If so, we can complete the subset by picking $k-1$ other items from the other $n-1$. If not, we must pick all k items from the remaining $n-1$. There is no overlap between these cases, and all possibilities are included, so the sum counts all k subsets.

No recurrence is complete without basis cases. What binomial coefficient values do we know without computing them? The left term of the sum eventually drives us down to $\binom{n-k}{0}$. How many ways are there to choose 0 things from a set? Exactly one, the empty set. If this is not convincing, then it is equally good to accept that $\binom{m}{1} = m$ as the basis case. The right term of the sum runs us up to $\binom{k}{k}$. How many ways are there to choose k things from a k-element set? Exactly one—the complete set. Together, these basis cases and the recurrence define the binomial coefficients on all interesting values.

The best way to evaluate such a recurrence is to build a table of possible values up to the size that you are interested in:

Figure 8.3 demonstrates a proper evaluation order for the recurrence. The initialized cells are marked from A-K, denoting the order in which they were assigned values. Each remaining cell is assigned the sum of the cell directly above it and the cell immediately above and to the left. The triangle of cells marked 1 to 10 denote the evaluation order in computing $\binom{5}{4} = 5$ using the code below:

```
long binomial_coefficient(n,m)
int n,m;                          /* computer n choose m */
{
        int i,j;                  /* counters */
        long bc[MAXN][MAXN];      /* table of binomial coefficients */

        for (i=0; i<=n; i++) bc[i][0] = 1;

        for (j=0; j<=n; j++) bc[j][j] = 1;

        for (i=1; i<=n; i++)
                for (j=1; j<i; j++)
                        bc[i][j] = bc[i-1][j-1] + bc[i-1][j];

        return( bc[n][m] );
}
```

Study this function carefully to see how we did it. The rest of this chapter will focus more on formulating and analyzing the appropriate recurrence than the mechanics of table manipulation demonstrated here.

8.2 Approximate String Matching

Searching for patterns in text strings is a problem of unquestionable importance. Section 3.7.2 (page 91) presented algorithms for *exact* string matching—finding where the pattern string P occurs as a substring of the text string T. Life is often not that simple. Words in either the text or pattern can be mispelled (sic), robbing us of exact similarity. Evolutionary changes in genomic sequences or language usage imply that we often search with archaic patterns in mind: "Thou shalt not kill" morphs over time into "You should not murder."

How can we search for the substring closest to a given pattern to compensate for spelling errors? To deal with inexact string matching, we must first define a cost function telling us how far apart two strings are—i.e., a distance measure between pairs of strings. A reasonable distance measure reflects the number of *changes* that must be made to convert one string to another. There are three natural types of changes:

- *Substitution* – Replace a single character from pattern P with a different character in text T, such as changing "shot" to "spot."
- *Insertion* – Insert a single character into pattern P to help it match text T, such as changing "ago" to "agog."
- *Deletion* – Delete a single character from pattern P to help it match text T, such as changing "hour" to "our."

Properly posing the question of string similarity requires us to set the cost of each of these string transform operations. Assigning each operation an equal cost of 1 defines the *edit distance* between two strings. Approximate string matching arises in many applications, as discussed in Section 18.4 (page 631).

Approximate string matching seems like a difficult problem, because we must decide exactly where to delete and insert (potentially) many characters in pattern and text. But let us think about the problem in reverse. What information would we like to have to make the final decision? What can happen to the last character in the matching for each string?

8.2.1 Edit Distance by Recursion

We can define a recursive algorithm using the observation that the last character in the string must either be matched, substituted, inserted, or deleted. Chopping off the characters involved in this last edit operation leaves a pair of smaller strings. Let i and j be the last character of the relevant prefix of P and T, respectively. There are three pairs of shorter strings after the last operation, corresponding to the strings after a match/substitution, insertion, or deletion. *If* we knew the cost of editing these three pairs of smaller strings, we could decide which option leads to the best solution and choose that option accordingly. We *can* learn this cost through the magic of recursion.

More precisely, let $D[i, j]$ be the minimum number of differences between $P_1, P_2, \ldots, P_i$ and the segment of T ending at j. $D[i, j]$ is the *minimum* of the three possible ways to extend smaller strings:

- If $(P_i = T_j)$, then $D[i-1, j-1]$, else $D[i-1, j-1]+1$. This means we either match or substitute the ith and jth characters, depending upon whether the tail characters are the same.

- $D[i-1, j]+1$. This means that there is an extra character in the pattern to account for, so we do not advance the text pointer and pay the cost of an insertion.

- $D[i, j-1]+1$. This means that there is an extra character in the text to remove, so we do not advance the pattern pointer and pay the cost of a deletion.

```
#define MATCH       0       /* enumerated type symbol for match */
#define INSERT      1       /* enumerated type symbol for insert */
#define DELETE      2       /* enumerated type symbol for delete */
```

```
int string_compare(char *s, char *t, int i, int j)
{
        int k;                  /* counter */
        int opt[3];             /* cost of the three options */
        int lowest_cost;        /* lowest cost */

        if (i == 0) return(j * indel(' '));
        if (j == 0) return(i * indel(' '));

        opt[MATCH] = string_compare(s,t,i-1,j-1) + match(s[i],t[j]);
        opt[INSERT] = string_compare(s,t,i,j-1) + indel(t[j]);
        opt[DELETE] = string_compare(s,t,i-1,j) + indel(s[i]);

        lowest_cost = opt[MATCH];
        for (k=INSERT; k<=DELETE; k++)
                if (opt[k] < lowest_cost) lowest_cost = opt[k];

        return( lowest_cost );
}
```

This program is absolutely correct—convince yourself. It also turns out to be impossibly slow. Running on my computer, the computation takes several seconds to compare two 11-character strings, and disappears into Never-Never Land on anything longer.

Why is the algorithm so slow? It takes exponential time because it recomputes values again and again and again. At every position in the string, the recursion branches three ways, meaning it grows at a rate of at least 3^n—indeed, even faster since most of the calls reduce only one of the two indices, not both of them.

8.2.2 Edit Distance by Dynamic Programming

So, how can we make this algorithm practical? The important observation is that most of these recursive calls are computing things that have been previously computed. How do we know? There can only be $|P| \cdot |T|$ possible unique recursive calls, since there are only that many distinct (i, j) pairs to serve as the argument parameters of recursive calls. By storing the values for each of these (i, j) pairs in a table, we just look them up as needed and avoid recomputing them.

A table-based, dynamic programming implementation of this algorithm is given below. The table is a two-dimensional matrix m where each of the $|P| \cdot |T|$ cells contains the cost of the optimal solution to a subproblem, as well as a parent pointer explaining how we got to this location:

```
typedef struct {
        int cost;               /* cost of reaching this cell */
        int parent;             /* parent cell */
} cell;

cell m[MAXLEN+1][MAXLEN+1];     /* dynamic programming table */
```

Our dynamic programming implementation has three differences from the recursive version. First, it gets its intermediate values using table lookup instead of recursive calls. Second, it updates the `parent` field of each cell, which will enable us to reconstruct the edit sequence later. Third, it is implemented using a more general `goal_cell()` function instead of just returning `m[|P|][|T|].cost`. This will enable us to apply this routine to a wider class of problems.

```
int string_compare(char *s, char *t)
{
        int i,j,k;              /* counters */
        int opt[3];             /* cost of the three options */

        for (i=0; i<MAXLEN; i++) {
                row_init(i);
                column_init(i);
        }

        for (i=1; i<strlen(s); i++) {
                for (j=1; j<strlen(t); j++) {
                        opt[MATCH] = m[i-1][j-1].cost + match(s[i],t[j]);
                        opt[INSERT] = m[i][j-1].cost + indel(t[j]);
                        opt[DELETE] = m[i-1][j].cost + indel(s[i]);

                        m[i][j].cost = opt[MATCH];
                        m[i][j].parent = MATCH;
                        for (k=INSERT; k<=DELETE; k++)
                                if (opt[k] < m[i][j].cost) {
                                        m[i][j].cost = opt[k];
                                        m[i][j].parent = k;
                                }
                }
        }
        goal_cell(s,t,&i,&j);
        return( m[i][j].cost );
}
```

P	T pos		y	o	u	-	s	h	o	u	l	d	-	n	o	t
		0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
:		**0**	1	2	3	4	5	6	7	8	9	10	11	12	13	14
t:	1	**1**	1	2	3	4	5	6	7	8	9	10	11	12	13	13
h:	2	2	**2**	2	3	4	5	5	6	7	8	9	10	11	12	13
o:	3	3	3	**2**	3	4	5	6	5	6	7	8	9	10	11	12
u:	4	4	4	3	**2**	3	4	5	6	5	6	7	8	9	10	11
-:	5	5	5	4	3	**2**	3	4	5	6	6	7	7	8	9	10
s:	6	6	6	5	4	3	**2**	3	4	5	6	7	8	8	9	10
h:	7	7	7	6	5	4	3	**2**	**3**	4	5	6	7	8	9	10
a:	8	8	8	7	6	5	4	3	3	**4**	5	6	7	8	9	10
l:	9	9	9	8	7	6	5	4	4	4	**4**	5	6	7	8	9
t:	10	10	10	9	8	7	6	5	5	5	5	**5**	6	7	8	8
-:	11	11	11	10	9	8	7	6	6	6	6	6	**5**	6	7	8
n:	12	12	12	11	10	9	8	7	7	7	7	7	6	**5**	6	7
o:	13	13	13	12	11	10	9	8	7	8	8	8	7	6	**5**	6
t:	14	14	14	13	12	11	10	9	8	8	9	9	8	7	6	**5**

Figure 8.4: Example of a dynamic programming matrix for editing distance computation, with the optimal alignment path highlighted in bold

Be aware that we adhere to somewhat unusual string and index conventions in the routine above. In particular, we assume that each string has been padded with an initial blank character, so the first real character of string `s` sits in `s[1]`. Why did we do this? It enables us to keep the matrix `m` indices in sync with those of the strings for clarity. Recall that we must dedicate the zeroth row and column of `m` to store the boundary values matching the empty prefix. Alternatively, we could have left the input strings intact and just adjusted the indices accordingly.

To determine the value of cell (i, j), we need three values sitting and waiting for us—namely, the cells $(i-1, j-1)$, $(i, j-1)$, and $(i-1, j)$. Any evaluation order with this property will do, including the row-major order used in this program.[1]

As an example, we show the cost matrices for turning p = "thou shalt not" into t = "you should not" in five moves in Figure 8.4.

8.2.3 Reconstructing the Path

The string comparison function returns the cost of the optimal alignment, but not the alignment itself. Knowing you can convert "thou shalt not" to "you should not" in only five moves is dandy, but what is the sequence of editing operations that does it?

The possible solutions to a given dynamic programming problem are described by paths through the dynamic programming matrix, starting from the initial configuration (the pair of empty strings $(0, 0)$) down to the final goal state (the pair

[1]Suppose we create a graph with a vertex for every matrix cell, and a directed edge (x, y), when the value of cell x is needed to compute the value of cell y. Any topological sort on the resulting DAG (why must it be a DAG?) defines an acceptable evaluation order.

P	T pos	0	y 1	o 2	u 3	- 4	s 5	h 6	o 7	u 8	l 9	d 10	- 11	n 12	o 13	t 14
	0	**-1**	1	1	1	1	1	1	1	1	1	1	1	1	1	1
t:	1	**2**	0	0	0	0	0	0	0	0	0	0	0	0	0	0
h:	2	2	**0**	0	0	0	0	0	1	1	1	1	1	1	1	1
o:	3	2	0	**0**	0	0	0	0	0	1	1	1	1	1	0	1
u:	4	2	0	2	**0**	1	1	1	1	0	1	1	1	1	1	1
-:	5	2	0	2	2	**0**	1	1	1	1	0	0	0	1	1	1
s:	6	2	0	2	2	2	**0**	1	1	1	1	0	0	0	0	0
h:	7	2	0	2	2	2	2	**0**	**1**	1	1	1	1	1	0	0
a:	8	2	0	2	2	2	2	2	0	**0**	0	0	0	0	0	0
l:	9	2	0	2	2	2	2	2	0	0	**0**	1	1	1	1	1
t:	10	2	0	2	2	2	2	2	0	0	0	**0**	0	0	0	0
-:	11	2	0	2	2	0	2	2	0	0	0	0	**0**	1	1	1
n:	12	2	0	2	2	2	2	2	0	0	0	0	2	**0**	1	1
o:	13	2	0	0	2	2	2	2	0	0	0	0	2	2	**0**	1
t:	14	2	0	2	2	2	2	2	2	0	0	0	2	2	2	**0**

Figure 8.5: Parent matrix for edit distance computation, with the optimal alignment path highlighted in bold

of full strings ($|P|, |T|$)). The key to building the solution is to reconstruct the decisions made at every step along the optimal path that leads to the goal state. These decisions have been recorded in the `parent` field of each array cell.

Reconstructing these decisions is done by walking backward from the goal state, following the `parent` pointer back to an earlier cell. We repeat this process until we arrive back at the initial cell. The `parent` field for `m[i,j]` tells us whether the operation at (i, j) was `MATCH`, `INSERT`, or `DELETE`. Tracing back through the parent matrix in Figure 8.5 yields the edit sequence `DSMMMMMISMSMMMM` from "thou-shalt-not" to "you-should-not"—meaning delete the first "t", replace the "h" with "y", match the next five characters before inserting an "o", replace "a" with "u", and finally replace the "t" with a "d."

Walking backward reconstructs the solution in reverse order. However, clever use of recursion can do the reversing for us:

```
reconstruct_path(char *s, char *t, int i, int j)
{
        if (m[i][j].parent == -1) return;

        if (m[i][j].parent == MATCH) {
                reconstruct_path(s,t,i-1,j-1);
                match_out(s, t, i, j);
                return;
        }
        if (m[i][j].parent == INSERT) {
                reconstruct_path(s,t,i,j-1);
                insert_out(t,j);
```

```
                return;
        }
        if (m[i][j].parent == DELETE) {
                reconstruct_path(s,t,i-1,j);
                delete_out(s,i);
                return;
        }
}
```

For many problems, including edit distance, the tour can be reconstructed from the cost matrix without explicitly retaining the last-move pointer array. The trick is working backward from the costs of the three possible ancestor cells and corresponding string characters to reconstruct the move that took you to the current cell at the given cost.

8.2.4 Varieties of Edit Distance

The `string_compare` and path reconstruction routines reference several functions that we have not yet defined. These fall into four categories:

- *Table Initialization* – The functions `row_init` and `column_init` initialize the zeroth row and column of the dynamic programming table, respectively. For the string edit distance problem, cells $(i, 0)$ and $(0, i)$ correspond to matching length-i strings against the empty string. This requires exactly i insertions/deletions, so the definition of these functions is clear:

```
row_init(int i)
{
 m[0][i].cost = i;
 if (i>0)
     m[0][i].parent =  INSERT;
 else
     m[0][i].parent = -1;
}
```

```
column_init(int i)
{
 m[i][0].cost = i;
 if (i>0)
     m[i][0].parent = DELETE;
 else
     m[i][0].parent = -1;
}
```

- *Penalty Costs* – The functions `match(c,d)` and `indel(c)` present the costs for transforming character c to d and inserting/deleting character c. For standard edit distance, `match` should cost nothing if the characters are identical, and 1 otherwise; while `indel` returns 1 regardless of what the argument is. But application-specific cost functions can be employed, perhaps more forgiving of replacements located near each other on standard keyboard layouts or characters that sound or look similar.

```
int match(char c, char d)
{
  if (c == d) return(0);
  else return(1);
}
```

```
int indel(char c)
{
  return(1);
}
```

- *Goal Cell Identification* – The function `goal_cell` returns the indices of the cell marking the endpoint of the solution. For edit distance, this is defined by the length of the two input strings. However, other applications we will soon encounter do not have fixed goal locations.

```
goal_cell(char *s, char *t, int *i, int *j)
{
  *i = strlen(s) - 1;
  *j = strlen(t) - 1;
}
```

- *Traceback Actions* – The functions `match_out`, `insert_out`, and `delete_out` perform the appropriate actions for each edit operation during traceback. For edit distance, this might mean printing out the name of the operation or character involved, as determined by the needs of the application.

```
insert_out(char *t, int j)
{
        printf("I");
}

delete_out(char *s, int i)
{
        printf("D");
}
```

```
match_out(char *s, char *t,
          int i, int j)
{
    if (s[i]==t[j]) printf("M");
    else printf("S");
}
```

All of these functions are quite simple for edit distance computation. However, we must confess it is difficult to get the boundary conditions and index manipulations correctly. Although dynamic programming algorithms are easy to design once you understand the technique, getting the details right requires carefully thinking and thorough testing.

This may seem to be a lot of infrastructure to develop for such a simple algorithm. However, several important problems can now be solved as special cases of edit distance using only minor changes to some of these stub functions:

- *Substring Matching* – Suppose that we want to find where a short pattern P best occurs within a long text T—say, searching for "Skiena" in all its misspellings (Skienna, Skena, Skina, ...) within a long file. Plugging this

search into our original edit distance function will achieve little sensitivity, since the vast majority of any edit cost will consist of deleting that which is not "Skiena" from the body of the text. Indeed, matching any scattered $\cdots S \cdots k \cdots i \cdots e \cdots n \cdots a$ and deleting the rest yields an optimal solution.

We want an edit distance search where the cost of starting the match is independent of the position in the text, so that a match in the middle is not prejudiced against. Now the goal state is not necessarily at the end of both strings, but the cheapest place to match the entire pattern somewhere in the text. Modifying these two functions gives us the correct solution:

```
row_init(int i)
{
        m[0][i].cost = 0;       /* note change */
        m[0][i].parent = -1;    /* note change */
}

goal_cell(char *s, char *t, int *i, int *j)
{
        int k;                  /* counter */

        *i = strlen(s) - 1;
        *j = 0;
        for (k=1; k<strlen(t); k++)
                if (m[*i][k].cost < m[*i][*j].cost) *j = k;
}
```

- *Longest Common Subsequence* – Perhaps we are interested in finding the longest scattered string of characters included within both strings. Indeed, this problem will be discussed in Section 18.8. The *longest common subsequence* (LCS) between "democrat" and "republican" is *eca*.

  A common subsequence is defined by all the identical-character matches in an edit trace. To maximize the number of such matches, we must prevent substitution of nonidentical characters. With substitution forbidden, the only way to get rid of the noncommon subsequence is through insertion and deletion. The minimum cost alignment has the fewest such "in-dels", so it must preserve the longest common substring. We get the alignment we want by changing the match-cost function to make substitutions expensive:

```
int match(char c, char d)
{
        if (c == d) return(0);
        else return(MAXLEN);
}
```

Actually, it suffices to make the substitution penalty greater than that of an insertion plus a deletion for substitution to lose any allure as a possible edit operation.

- *Maximum Monotone Subsequence* – A numerical sequence is *monotonically increasing* if the ith element is at least as big as the $(i-1)$st element. The *maximum monotone subsequence* problem seeks to delete the fewest number of elements from an input string S to leave a monotonically increasing subsequence. A longest increasing subsequence of 243517698 is 23568.

  In fact, this is just a longest common subsequence problem, where the second string is the elements of S sorted in increasing order. Any common sequence of these two must (a) represent characters in proper order in S, and (b) use only characters with increasing position in the collating sequence—so, the longest one does the job. Of course, this approach can be modified to give the longest decreasing sequence by simply reversing the sorted order.

As you can see, our edit distance routine can be made to do many amazing things easily. The trick is observing that your problem is just a special case of approximate string matching.

The alert reader may notice that it is unnecessary to keep all $O(mn)$ cells to compute the cost of an alignment. If we evaluate the recurrence by filling in the columns of the matrix from left to right, we will never need more than two columns of cells to store what is necessary for the computation. Thus, $O(m)$ space is sufficient to evaluate the recurrence without changing the time complexity. Unfortunately, we cannot reconstruct the alignment without the full matrix.

Saving space in dynamic programming is very important. Since memory on any computer is limited, using $O(nm)$ space proves more of a bottleneck than $O(nm)$ time. Fortunately, there is a clever divide-and-conquer algorithm that computes the actual alignment in $O(nm)$ time and $O(m)$ space. It is discussed in Section 18.4 (page 631).

8.3 Longest Increasing Sequence

There are three steps involved in solving a problem by dynamic programming:

1. Formulate the answer as a recurrence relation or recursive algorithm.
2. Show that the number of different parameter values taken on by your recurrence is bounded by a (hopefully small) polynomial.
3. Specify an order of evaluation for the recurrence so the partial results you need are always available when you need them.

To see how this is done, let's see how we would develop an algorithm to find the longest monotonically increasing subsequence within a sequence of n numbers. Truth be told, this was described as a special case of edit distance in the previous section, where it was called *maximum monotone subsequence*. Still, it is instructive to work it out from scratch. Indeed, dynamic programming algorithms are often easier to reinvent than look up.

We distinguish an increasing sequence from a *run*, where the elements must be physical neighbors of each other. The selected elements of both must be sorted in increasing order from left to right. For example, consider the sequence

$$S = \{2, 4, 3, 5, 1, 7, 6, 9, 8\}$$

The longest increasing subsequence of S has length 5, including {2,3,5,6,8}. In fact, there are eight of this length (can you enumerate them?). There are four longest increasing runs of length 2: $(2, 4)$, $(3, 5)$, $(1, 7)$, and $(6, 9)$.

Finding the longest increasing run in a numerical sequence is straightforward. Indeed, you should be able to devise a linear-time algorithm fairly easily. But finding the longest increasing subsequence is considerably trickier. How can we identify which scattered elements to skip? To apply dynamic programming, we need to construct a recurrence that computes the length of the longest sequence. To find the right recurrence, ask what information about the first $n - 1$ elements of S would help you to find the answer for the entire sequence?

- The length of the longest increasing sequence in $s_1, s_2, \ldots, s_{n-1}$ seems a useful thing to know. In fact, this will be the longest increasing sequence in S, unless s_n extends some increasing sequence of the same length.

  Unfortunately, the length of this sequence is not enough information to complete the full solution. Suppose I told you that the longest increasing sequence in $s_1, s_2, \ldots, s_{n-1}$ was of length 5 and that $s_n = 9$. Will the length of the final longest increasing subsequence of S be 5 or 6?

- We need to know the length of the longest sequence that s_n will extend. To be certain we know this, we really need the length of the longest sequence that *any* possible value for s_n can extend.

This provides the idea around which to build a recurrence. Define l_i to be the length of the longest sequence ending with s_i.

The longest increasing sequence containing the nth number will be formed by appending it to the longest increasing sequence to the left of n that ends on a number smaller than s_n. The following recurrence computes l_i:

$$\begin{aligned} l_i &= \max_{0<j<i} l_j + 1, \text{ where } (s_j < s_i), \\ l_0 &= 0 \end{aligned}$$

These values define the length of the longest increasing sequence ending at each number. The length of the longest increasing subsequence of the entire permutation is given by $\max_{1 \leq i \leq n} l_i$, since the winning sequence will have to end somewhere.

Here is the table associated with our previous example:

Sequence s_i	2	4	3	5	1	7	6	9	8
Length l_i	1	2	3	3	1	4	4	5	5
Predecessor p_i	–	1	1	2	–	4	4	6	6

What auxiliary information will we need to store to reconstruct the actual sequence instead of its length? For each element s_i, we will store its *predecessor*—the index p_i of the element that appears immediately before s_i in the longest increasing sequence ending at s_i. Since all of these pointers go towards the left, it is a simple matter to start from the last value of the longest sequence and follow the pointers so as to reconstruct the other items in the sequence.

What is the time complexity of this algorithm? Each one of the n values of l_i is computed by comparing s_i against (up to) $i - 1 \leq n$ values to the left of it, so this analysis gives a total of $O(n^2)$ time. In fact, by using dictionary data structures in a clever way, we can evaluate this recurrence in $O(n \lg n)$ time. However, the simple recurrence would be easy to program and therefore is a good place to start.

Take-Home Lesson: Once you understand dynamic programming, it can be easier to work out such algorithms from scratch than to try to look them up.

8.4 War Story: Evolution of the Lobster

I caught the two graduate students lurking outside my office as I came in to work that morning. There they were, two future PhDs working in the field of high-performance computer graphics. They studied new techniques for rendering pretty computer images, but the picture they painted for me that morning was anything but pretty.

"You see, we want to build a program to morph one image into another," they explained.

"What do you mean by morph?" I asked.

"For special effects in movies, we want to construct the intermediate stages in transforming one image into another. Suppose we want to turn you into Humphrey Bogart. For this to look realistic, we must construct a bunch of in-between frames that start out looking like you and end up looking like him."

"If you can realistically turn me into Bogart, you have something," I agreed.

"But our problem is that it isn't very realistic." They showed me a dismal morph between two images. "The trouble is that we must find the right corre-

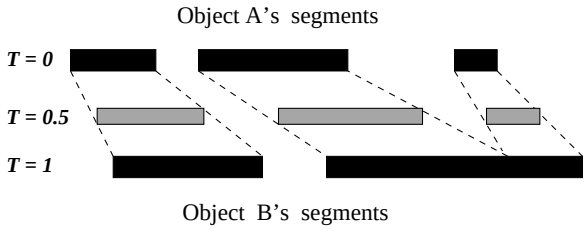

Figure 8.6: A successful alignment of two lines of pixels

spondence between features in the two images. It looks real bad when we get the correspondence wrong and try to morph a lip into an ear."

"I'll bet. So you want me to give you an algorithm for matching up lips?"

"No, even simpler. We morph each row of the initial image into the identical row of the final image. You can assume that we give you two lines of pixels, and you have to find the best possible match between the dark pixels in a row from object A to the dark pixels in the corresponding row of object B. Like this," they said, showing me images of successful matchings like Figure 8.6.

"I see," I said. "You want to match big dark regions to big dark regions and small dark regions to small dark regions."

"Yes, but only if the matching doesn't shift them too much to the left or the right. We might prefer to merge or break up regions rather than shift them too far away, since that might mean matching a chin to an eyebrow. What is the best way to do it?"

"One last question. Will you ever want to match two intervals to each other in such a way that they cross?"

"No, I guess not. Crossing intervals can't match. It would be like switching your left and right eyes."

I scratched my chin and tried to look puzzled, but I'm just not as good an actor as Bogart. I'd had a hunch about what needed to be done the instant they started talking about lines of pixels. They want to transform one array of pixels into another array, using the minimum amount of changes. That sounded like editing one string of pixels into another string, which is a classic application of dynamic programming. See Sections 8.2 and 18.4 for discussions of approximate string matching.

The fact that the intervals couldn't cross settled the issue. It meant that whenever a stretch of dark pixels from A was mapped to a stretch from B, the problem would be split into two smaller subproblems—i.e. , the pixels to the left of the match and the pixels to the right of the match. The cost of the global match would ultimately be the cost of this match plus those of matching all the pixels to the left and of matching all the pixels to the right. Constructing the optimal match on the left side is a smaller problem and hence simpler. Further, there could be only

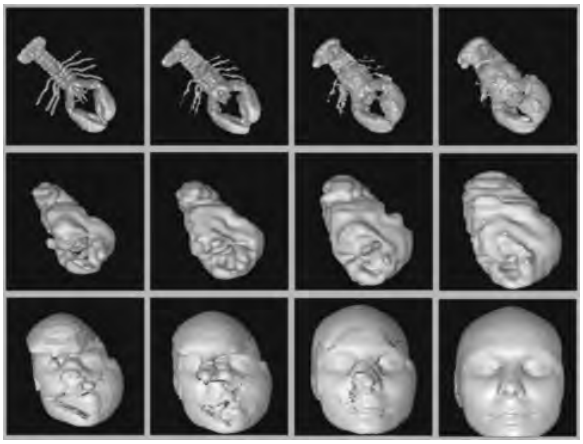

Figure 8.7: Morphing a lobster into a head via dynamic programming

$O(n^2)$ possible left subproblems, since each is completely described by the pair of one of n top pixels and one of n bottom pixels.

"Your algorithm will be based on dynamic programming," I pronounced. "However, there are several possible ways to do things, depending upon whether you want to edit pixels or runs. I would probably convert each row into a list of black pixel runs, with the runs sorted by right endpoint. Label each run with its starting position and length. You will maintain the cost of the cheapest match between the leftmost i runs and the leftmost j runs for all i and j. The possible edit operations are:

- *Full run match* – We may match top run i to run bottom j for a cost that is a function of the difference in the lengths of the two runs and their positions.

- *Merging runs* – We may match a string of consecutive top runs to a bottom run. The cost will be a function of the number of runs, their relative positions, and their lengths.

- *Splitting runs* – We may match a top run to a string of consecutive bottom runs. This is just the converse of the merge. Again, the cost will be a function of the number of runs, their relative positions, and their lengths.

"For each pair of runs (i, j) and all the cases that apply, we compute the cost of the edit operation and add to the (already computed and stored) edit cost to the left of the start of the edit. The cheapest of these cases is what we will take for the cost of $c[i, j]$."

The pair of graduate students scribbled this down, then frowned. "So we will have a cost measure for matching two runs as a function of their lengths and positions. How do we decide what the relative costs should be?"

"That is your business. The dynamic programming serves to optimize the matchings *once* you know the cost functions. It is up to your aesthetic sense to decide the penalties for line length changes and offsets. My recommendation is that you implement the dynamic programming and try different penalty values on each of several different images. Then, pick the setting that seems to do what you want."

They looked at each other and smiled, then ran back into the lab to implement it. Using dynamic programming to do their alignments, they completed their morphing system. It produced the images in Figure 8.7, morphing a lobster into a man. Unfortunately, they never got around to turning me into Humphrey Bogart.

8.5 The Partition Problem

Suppose that three workers are given the task of scanning through a shelf of books in search of a given piece of information. To get the job done fairly and efficiently, the books are to be partitioned among the three workers. To avoid the need to rearrange the books or separate them into piles, it is simplest to divide the shelf into three regions and assign each region to one worker.

But what is the fairest way to divide up the shelf? If all books are the same length, the job is pretty easy. Just partition the books into equal-sized regions,

100 100 100 | 100 100 100 | 100 100 100

so that everyone has 300 pages to deal with.

But what if the books are not the same length? Suppose we used the same partition when the book sizes looked like this:

100 200 300 | 400 500 600 | 700 800 900

I, would volunteer to take the first section, with only 600 pages to scan, instead of the last one, with 2,400 pages. The fairest possible partition for this shelf would be

100 200 300 400 500 | 600 700 | 800 900

where the largest job is only 1,700 pages and the smallest job 1,300.

In general, we have the following problem:

Problem: Integer Partition without Rearrangement
Input: An arrangement S of nonnegative numbers $\{s_1, \ldots, s_n\}$ and an integer k.
Output: Partition S into k or fewer ranges, to minimize the maximum sum over all the ranges, without reordering any of the numbers.

This so-called *linear partition* problem arises often in parallel process. We seek to balance the work done across processors to minimize the total elapsed run time.

The bottleneck in this computation will be the processor assigned the most work. Indeed, the war story of Section 7.10 (page 268) revolves around a botched solution to this problem.

Stop for a few minutes and try to find an algorithm to solve the linear partition problem.

A novice algorist might suggest a heuristic as the most natural approach to solving the partition problem. Perhaps they would compute the average size of a partition, $\sum_{i=1}^{n} s_i/k$, and then try to insert the dividers to come close to this average. However, such heuristic methods are doomed to fail on certain inputs because they do not systematically evaluate all possibilities.

Instead, consider a recursive, exhaustive search approach to solving this problem. Notice that the kth partition starts right after we placed the $(k-1)$st divider. Where can we place this last divider? Between the ith and $(i+1)$st elements for some i, where $1 \leq i \leq n$. What is the cost of this? The total cost will be the larger of two quantities—(1) the cost of the last partition $\sum_{j=i+1}^{n} s_j$, and (2) the cost of the largest partition formed to the left of i. What is the size of this left partition? To minimize our total, we want to use the $k-2$ remaining dividers to partition the elements $\{s_1, \ldots, s_i\}$ as equally as possible. *This is a smaller instance of the same problem, and hence can be solved recursively!*

Therefore, let us define $M[n,k]$ to be the minimum possible cost over all partitionings of $\{s_1, \ldots, s_n\}$ into k ranges, where the cost of a partition is the largest sum of elements in one of its parts. Thus defined, this function can be evaluated:

$$M[n,k] = \min_{i=1}^{n} \max(M[i,k-1], \sum_{j=i+1}^{n} s_j)$$

We must specify the boundary conditions of the recurrence relation. These boundary conditions always settle the smallest possible values for each of the arguments of the recurrence. For this problem, the smallest reasonable value of the first argument is $n = 1$, meaning that the first partition consists of a single element. We can't create a first partition smaller than s_1 regardless of how many dividers are used. The smallest reasonable value of the second argument is $k = 1$, implying that we do not partition S at all. In summary:

$$M[1,k] = s_1, \text{ for all } k > 0 \text{ and,}$$

$$M[n,1] = \sum_{i=1}^{n} s_i$$

By definition, this recurrence must return the size of the optimal partition. How long does it take to compute this when we store the partial results? A total of $k \cdot n$ cells exist in the table. How much time does it take to compute the result

$M[n', k']$? Calculating this quantity involves finding the minimum of n' quantities, each of which is the maximum of the table lookup and a sum of at most n' elements. If filling each of kn boxes takes at most n^2 time per box, the total recurrence can be computed in $O(kn^3)$ time.

The evaluation order computes the smaller values before the bigger values, so that each evaluation has what it needs waiting for it. Full details are provided in the code below:

```
partition(int s[], int n, int k)
{
        int m[MAXN+1][MAXK+1];                  /* DP table for values */
        int d[MAXN+1][MAXK+1];                  /* DP table for dividers */
        int p[MAXN+1];                          /* prefix sums array */
        int cost;                               /* test split cost */
        int i,j,x;                              /* counters */

        p[0] = 0;                               /* construct prefix sums */
        for (i=1; i<=n; i++) p[i]=p[i-1]+s[i];

        for (i=1; i<=n; i++) m[i][1] = p[i];    /* initialize boundaries */
        for (j=1; j<=k; j++) m[1][j] = s[1];

        for (i=2; i<=n; i++)                    /* evaluate main recurrence */
                for (j=2; j<=k; j++) {
                        m[i][j] = MAXINT;
                        for (x=1; x<=(i-1); x++) {
                                cost = max(m[x][j-1], p[i]-p[x]);
                                if (m[i][j] > cost) {
                                        m[i][j] = cost;
                                        d[i][j] = x;
                                }
                        }
                }

        reconstruct_partition(s,d,n,k);         /* print book partition */
}
```

This implementation above, in fact, runs faster than advertised. Our original analysis assumed that it took $O(n^2)$ time to update each cell of the matrix. This is because we selected the best of up to n possible points to place the divider, each of which requires the sum of up to n possible terms. In fact, it is easy to avoid the need to compute these sums by storing the set of n prefix sums $p[i] = \sum_{k=1}^{i} s_k$,

M	k		
n	1	2	3
1	1	1	1
1	2	1	1
1	3	2	1
1	4	2	2
1	5	3	2
1	6	3	2
1	7	4	3
1	8	4	3
1	9	5	3

D	k		
n	1	2	3
1	–	–	–
1	–	1	1
1	–	1	2
1	–	2	2
1	–	2	3
1	–	3	4
1	–	3	4
1	–	4	5
1	–	4	6

M	k		
n	1	2	3
1	1	1	1
2	3	2	2
3	6	3	3
4	10	6	4
5	15	9	6
6	21	11	9
7	28	15	11
8	36	21	15
9	45	24	17

D	k		
n	1	2	3
1	–	–	–
2	–	1	1
3	–	2	2
4	–	3	3
5	–	3	4
6	–	4	5
7	–	5	6
8	–	5	6
9	–	6	7

Figure 8.8: Dynamic programming matrices M and D for two input instances. Partitioning $\{1,1,1,1,1,1,1,1,1\}$ into $\{\{1,1,1\},\{1,1,1\},\{1,1,1\}\}$ (l) . Partitioning $\{1,2,3,4,5,6,7,8,9\}$ into $\{\{1,2,3,4,5\},\{6,7\},\{8,9\}\}$ (r).

since $\sum_{k=i}^{j} s_k = p[j] - p[k]$. This enables us to evaluate the recurrence in linear time per cell, yielding an $O(kn^2)$ algorithm.

By studying the recurrence relation and the dynamic programming matrices of Figure 8.8, you should be able to convince yourself that the final value of $M(n,k)$ will be the cost of the largest range in the optimal partition. For most applications, however, what we need is the actual partition that does the job. Without it, all we are left with is a coupon with a great price on an out-of-stock item.

The second matrix, D, is used to reconstruct the optimal partition. Whenever we update the value of $M[i,j]$, we record which divider position was required to achieve that value. To reconstruct the path used to get to the optimal solution, we work backward from $D[n,k]$ and add a divider at each specified position. This backwards walking is best achieved by a recursive subroutine:

```
reconstruct_partition(int s[],int d[MAXN+1][MAXK+1], int n, int k)
{
        if (k==1)
                print_books(s,1,n);
        else {
                reconstruct_partition(s,d,d[n][k],k-1);
                print_books(s,d[n][k]+1,n);
        }
}


print_books(int s[], int start, int end)
{
        int i;                  /* counter */

        for (i=start; i<=end; i++) printf(" %d ",s[i]);
        printf("\n");
}
```

sentence ::= noun−phrase
verb−phrase
noun−phrase ::= article noun
verb−phrase ::= verb noun−phrase
article ::= *the, a*
noun ::= *cat, milk*
verb ::= *drank*

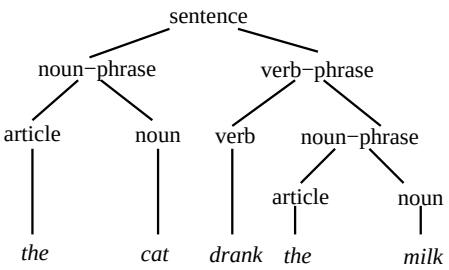

Figure 8.9: A context-free grammar (l) with an associated parse tree (r)

8.6 Parsing Context-Free Grammars

Compilers identify whether the given program is legal in the programming language, and reward you with syntax errors if not. This requires a precise description of the language syntax typically given by a *context-free grammar* as shown in Figure 8.9(l). Each *rule* or *production* of the grammar defines an interpretation for the named symbol on the left side of the rule as a sequence of symbols on the right side of the rule. The right side can be a combination of *nonterminals* (themselves defined by rules) or *terminal* symbols defined simply as strings, such as "the", "a", "cat", "milk", and "drank."

Parsing a given text string S according to a given context-free grammar G is the algorithmic problem of constructing a *parse tree* of rule substitutions defining S as a single nonterminal symbol of G. Figure 8.9(r) gives the parse tree of a simple sentence using our sample grammar.

Parsing seemed like a horribly complicated subject when I took a compilers course as a graduate student. But, a friend easily explained it to me over lunch a few years ago. The difference is that I now understand dynamic programming much better than when I was a student.

We assume that the text string S has length n while the grammar G itself is of constant size. This is fair, since the grammar defining a particular programming language (say C or Java) is of fixed length regardless of the size of the program we are trying to compile.

Further, we assume that the definitions of each rule are in *Chomsky normal form*. This means that the right sides of every nontrivial rule consists of (a) exactly two nonterminals, i.e. $X \rightarrow YZ$, or (b) exactly one terminal symbol, $X \rightarrow \alpha$. Any context-free grammar can be easily and mechanically transformed into Chomsky normal form by repeatedly shortening long right-hand sides at the cost of adding extra nonterminals and productions. Thus, there is no loss of generality with this assumption.

So how can we efficiently parse a string S using a context-free grammar where each interesting rule consists of two nonterminals? The key observation is that the rule applied at the root of the parse tree (say $X \rightarrow YZ$) splits S at some position i such that the left part of the string ($S[1, i]$) must be *generated* by nonterminal Y, and the right part ($S[i+1, n]$) generated by Z.

This suggests a dynamic programming algorithm, where we keep track of all of the nonterminals generated by each substring of S. Define $M[i, j, X]$ to be a boolean function that is true iff substring $S[i, j]$ is generated by nonterminal X. This is true if there exists a production $X \rightarrow YZ$ and breaking point k between i and j such that the left part generates Y and the right part Z. In other words,

$$M[i, j, X] = \bigvee_{(X \rightarrow YZ) \in G} \left(\bigvee_{i=k}^{j} M[i, k, Y] \cdot M[k+1, j, Z] \right)$$

where $\vee$ denotes the logical *or* over all productions and split positions, and $\cdot$ denotes the logical *and* of two boolean values.

The one-character terminal symbols define the boundary conditions of the recurrence. In particular, $M[i, i, X]$ is true iff there exists a production $X \rightarrow \alpha$ such that $S[i] = \alpha$.

What is the complexity of this algorithm? The size of our state-space is $O(n^2)$, as there are $n(n+1)/2$ substrings defined by (i, j) pairs. Multiplying this by the number of nonterminals (say v) has no impact on the big-Oh, because the grammar was defined to be of constant size. Evaluating the value $M[i, j, X]$ requires testing all intermediate values k, so it takes $O(n)$ in the worst case to evaluate each of the $O(n^2)$ cells. This yields an $O(n^3)$ or cubic-time algorithm for parsing.

Stop and Think: Parsimonious Parserization

Problem: Programs often contain trivial syntax errors that prevent them from compiling. Given a context-free grammar G and input string S, find the smallest number of character substitutions you must make to S so that the resulting string is accepted by G.

Solution: This problem seemed extremely difficult when I first encountered it. But on reflection, it seemed like a very general version of edit distance, which is addressed naturally by dynamic programming. Parsing initially sounded hard, too, but fell to the same technique. Indeed, we can solve the combined problem by generalizing the recurrence relation we used for simple parsing.

Define $M'[i, j, X]$ to be an *integer* function that reports the minimum number of changes to substring $S[i, j]$ so it can be generated by nonterminal X. This symbol will be generated by some production $x \rightarrow yz$. Some of the changes to s may be

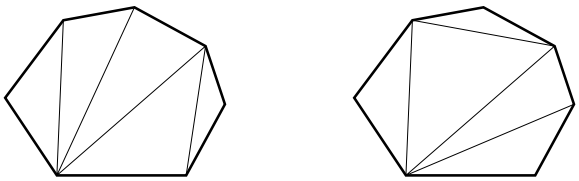

Figure 8.10: Two different triangulations of a given convex seven-gon

to the left of the breaking point and some to the right, but all we care about is minimizing the sum. In other words,

$$M'[i,j,X] = \min_{(X \to YZ) \in G} \left(\min_{i=k}^{j} M'[i,k,Y] + M'[k+1,j,Z] \right)$$

The boundary conditions also change mildly. If there exists a production $X \to \alpha$, the cost of matching at position i depends on the contents of $S[i]$, where $S[i] = \alpha$, $M[i,i,X] = 0$. Otherwise, it is one substitution away, so $M[i,i,X] = 1$ if $S[i] \neq \alpha$. If the grammar does not have a production of the form $X \to \alpha$, there is no way to substitute a single character string into something generating X, so $M[i,i,X] = \infty$ for all i. ∎

8.6.1 Minimum Weight Triangulation

The same basic recurrence relation encountered in the parsing algorithm above can also be used to solve an interesting computational geometry problem. A *triangulation* of a polygon $P = \{v_1, \ldots, v_n, v_1\}$ is a set of nonintersecting diagonals that partitions the polygon into triangles. We say that the *weight* of a triangulation is the sum of the lengths of its diagonals. As shown in Figure 8.10, any given polygon may have many different triangulations. We seek to find its minimum weight triangulation for a given polygon p. Triangulation is a fundamental component of most geometric algorithms, as discussed in Section 17.3 (page 572).

To apply dynamic programming, we need a way to carve up the polygon into smaller pieces. Observe that every edge of the input polygon must be involved in exactly one triangle. Turning this edge into a triangle means identifying the third vertex, as shown in Figure 8.11. Once we find the correct connecting vertex, the polygon will be partitioned into two smaller pieces, both of which need to be triangulated optimally. Let $T[i,j]$ be the cost of triangulating from vertex v_i to vertex v_j, ignoring the length of the chord d_{ij} from v_i to v_j. The latter clause avoids double counting these internal chords in the following recurrence:

$$T[i,j] \quad = \quad \min_{k=i+1}^{j-1} (T[i,k] + T[k,j] + d_{ik} + d_{kj})$$

The basis condition applies when i and j are immediate neighbors, as $T[i,i+1] = 0$.

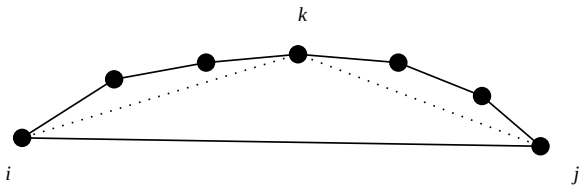

Figure 8.11: Selecting the vertex k to pair with an edge (i, j) of the polygon

Since the number of vertices in each subrange of the right side of the recurrence is smaller than that on the left side, evaluation can proceed in terms of the gap size from i to j:

```
Minimum-Weight-Triangulation(P)
    for i = 1 to n − 1 do T[i, i + 1] = 0
    for gap = 2 to n − 1
        for i = 1 to n − gap do
            j = i + gap
            T[i, j] = min_{k=i+1}^{j−1} (T[i, k] + T[k, j] + d_{P_i,P_k} + d_{P_k,P_j})
    return T[1, n]
```

There are $\binom{n}{2}$ values of T, each of which takes $O(j - i)$ time if we evaluate the sections in order of increasing size. Since $j - i = O(n)$, complete evaluation takes $O(n^3)$ time and $O(n^2)$ space.

What if there are points in the interior of the polygon? Then dynamic programming does not apply in the same way, because triangulation edges do not necessarily cut the boundary into two distinct pieces as before. Instead of only $\binom{n}{2}$ possible subregions, the number of subregions now grows exponentially. In fact, the more general version of this problem is known to be NP-complete.

Take-Home Lesson: For any optimization problem on left-to-right objects, such as characters in a string, elements of a permutation, points around a polygon, or leaves in a search tree, dynamic programming likely leads to an efficient algorithm to find the optimal solution.

8.7 Limitations of Dynamic Programming: TSP

Dynamic programming doesn't always work. It is important to see why it can fail, to help avoid traps leading to incorrect or inefficient algorithms.

Our algorithmic poster child will once again be the traveling salesman, where we seek the shortest tour visiting all the cities in a graph. We will limit attention here to an interesting special case:

Problem: Longest Simple Path
Input: A weighted graph G, with specified start and end vertices s and t.
Output: What is the most expensive path from s to t that does not visit any vertex more than once?

This problem differs from TSP in two quite unimportant ways. First, it asks for a path instead of a closed tour. This difference isn't substantial: we get a closed tour by simply including the edge (t, s). Second, it asks for the most expensive path instead of the least expensive tour. Again this difference isn't very significant: it encourages us to visit as many vertices as possible (ideally all), just as in TSP. The big word in the problem statement is *simple*, meaning we are not allowed to visit any vertex more than once.

For *unweighted* graphs (where each edge has cost 1), the longest possible simple path from s to t is $n - 1$. Finding such *Hamiltonian paths* (if they exist) is an important graph problem, discussed in Section 16.5 (page 538).

8.7.1 When are Dynamic Programming Algorithms Correct?

Dynamic programming algorithms are only as correct as the recurrence relations they are based on. Suppose we define $LP[i, j]$ as a function denoting the length of the longest simple path from i to j. Note that the longest simple path from i to j had to visit some vertex x right before reaching j. Thus, the last edge visited must be of the form (x, j). This suggests the following recurrence relation to compute the length of the longest path, where $c(x, j)$ is the cost/weight of edge (x, j):

$$LP[i, j] = \max_{(x,j) \in E} LP[i, x] + c(x, j)$$

The idea seems reasonable, but can you see the problem? I see at least two of them.

First, this recurrence does nothing to enforce simplicity. How do we know that vertex j has not appeared previously on the longest simple path from i to x? If it did, adding the edge (x, j) will create a cycle. To prevent such a thing, we must define a different recursive function that explicitly remembers where we have been. Perhaps we could define $LP'[i, j, k]$ to be the function denoting the length of the longest path from i to j avoiding vertex k? This would be a step in the right direction, but still won't lead to a viable recurrence.

A second problem concerns evaluation order. What can you evaluate first? Because there is no left-to-right or smaller-to-bigger ordering of the vertices on the graph, it is not clear what the *smaller* subprograms are. Without such an ordering, we get are stuck in an infinite loop as soon as we try to do anything.

Dynamic programming can be applied to any problem that observes the *principle of optimality*. Roughly stated, this means that partial solutions can be optimally extended with regard to the *state* after the partial solution, instead of the specifics of the partial solution itself. For example, in deciding whether to extend an approximate string matching by a substitution, insertion, or deletion, we did not need to

know which sequence of operations had been performed to date. In fact, there may be several different edit sequences that achieve a cost of C on the first p characters of pattern P and t characters of string T. Future decisions are made based on the *consequences* of previous decisions, not the actual decisions themselves.

Problems do not satisfy the principle of optimality when the specifics of the operations matter, as opposed to just the cost of the operations. Such would be the case with a form of edit distance where we are not allowed to use combinations of operations in certain particular orders. Properly formulated, however, many combinatorial problems respect the principle of optimality.

8.7.2 When are Dynamic Programming Algorithms Efficient?

The running time of any dynamic programming algorithm is a function of two things: (1) number of partial solutions we must keep track of, and (2) how long it take to evaluate each partial solution. The first issue—namely the size of the state space—is usually the more pressing concern.

In all of the examples we have seen, the partial solutions are completely described by specifying the stopping *places* in the input. This is because the combinatorial objects being worked on (strings, numerical sequences, and polygons) have an implicit order defined upon their elements. This order cannot be scrambled without completely changing the problem. Once the order is fixed, there are relatively few possible stopping places or states, so we get efficient algorithms.

When the objects are not firmly ordered, however, we get an exponential number of possible partial solutions. Suppose the state of our partial solution is entire path P taken from the start to end vertex. Thus $LP[i, j, P]$ denotes the longest simple path from i to j, where P is the exact sequence of intermediate vertices between i and j on this path. The following recurrence relation works to compute this, where $P + x$ denotes appending x to the end of P:

$$LP[i, j, P + x] = \max_{(x,j) \in E, x, j \notin P} LP[i, x, P] + c(x, j)$$

This formulation is correct, but how efficient is it? The path P consists of an ordered sequence of up to $n - 3$ vertices. There can be up to $(n - 3)!$ such paths! Indeed, this algorithm is really using combinatorial search (*a la* backtracking) to construct all the possible intermediate paths. In fact, the max is somewhat misleading, as there can only be one value of x and one value of P to construct the state $LP[i, j, P + x]$.

We can do something better with this idea, however. Let $LP'[i, j, S]$ denote the longest simple path from i to j, where the intermediate vertices on this path are exactly those in the *subset* S. Thus, if $S = \{a, b, c\}$, there are exactly six paths consistent with S: *iabcj*, *iacbj*, *ibacj*, *ibcaj*, *icabj*, and *icbaj*. This state space is at most 2^n, and thus smaller than enumerating the paths. Further, this function can be evaluated using the following recurrence relation:

$$LP'[i, j, S \cup \{x\}] = \max_{(x,j) \in E, x, j \notin S} LP[i, x, S] + c(x, j)$$

where $S \cup \{x\}$ denotes unioning S with x.

The longest simple path from i to j can then be found by maximizing over all possible intermediate vertex subsets:

$$LP[i,j] = \max_S LP'[i,j,S]$$

There are only 2^n subsets of n vertices, so this is a big improvement over enumerating all $n!$ tours. Indeed, this method could certainly be used to solve TSPs for up to thirty vertices or so, where $n = 20$ would be impossible using the $O(n!)$ algorithm. Still, dynamic programming is most effective on well-ordered objects.

Take-Home Lesson: Without an inherent left-to-right ordering on the objects, dynamic programming is usually doomed to require exponential space and time.

8.8 War Story: What's Past is Prolog

"But our heuristic works very, very well in practice." My colleague was simultaneously boasting and crying for help.

Unification is the basic computational mechanism in logic programming languages like Prolog. A Prolog program consists of a set of rules, where each rule has a head and an associated action whenever the rule head matches or unifies with the current computation.

An execution of a Prolog program starts by specifying a goal, say $p(a, X, Y)$, where a is a constant and X and Y are variables. The system then systematically matches the head of the goal with the head of each of the rules that can be *unified* with the goal. Unification means binding the variables with the constants, if it is possible to match them. For the nonsense program below, $p(X, Y, a)$ unifies with either of the first two rules, since X and Y can be bound to match the extra characters. The goal $p(X, X, a)$ would only match the first rule, since the variable bound to the first and second positions must be the same.

$$p(a,a,a) := h(a);$$
$$p(b,a,a) := h(a) * h(b);$$
$$p(c,b,b) := h(b) + h(c);$$
$$p(d,b,b) := h(d) + h(b);$$

"In order to speed up unification, we want to preprocess the set of rule heads so that we can quickly determine which rules match a given goal. We must organize the rules in a trie data structure for fast unification."

Tries are extremely useful data structures in working with strings, as discussed in Section 12.3 (page 377). Every leaf of the trie represents one string. Each node on the path from root to leaf is labeled with exactly one character of the string, with the ith node of the path corresponding to the ith character of the string.

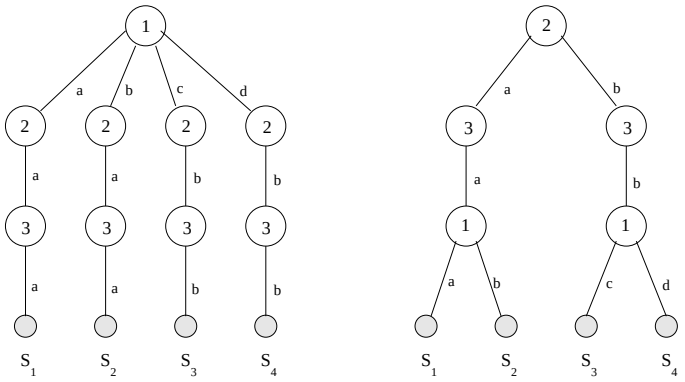

Figure 8.12: Two different tries for the same set of rule heads.

"I agree. A trie is a natural way to represent your rule heads. Building a trie on a set of strings of characters is straightforward: just insert the strings starting from the root. So what is your problem?" I asked.

"The efficiency of our unification algorithm depends very much on minimizing the number of edges in the trie. Since we know all the rules in advance, we have the freedom to reorder the character positions in the rules. Instead of the root node always representing the first argument in the rule, we can choose to have it represent the third argument. We would like to use this freedom to build a minimum-size trie for a set of rules."

He showed me the example in Figure 8.12. A trie constructed according to the original string position order $(1, 2, 3)$ uses a total of 12 edges. However, by permuting the character order to $(2, 3, 1)$, we can obtain a trie with only 8 edges.

"Interesting..." I started to reply before he cut me off again.

"There's one other constraint. We must keep the leaves of the trie ordered, so that the leaves of the underlying tree go left-to-right in the same order as the rules appear on the page."

"But why must you keep the leaves of the trie in the given order?" I asked.

"The order of rules in Prolog programs is very, very important. If you change the order of the rules, the program returns different results."

Then came my mission.

"We have a greedy heuristic for building good, but not optimal, tries based on picking as the root the character position that minimizes the degree of the root. In other words, it picks the character position that has the smallest number of distinct characters in it. This heuristic works very, very well in practice. But we need you to prove that finding the best trie is NP-complete so our paper is, well, complete."

I agreed to try to prove the hardness of the problem, and chased him from my office. The problem did seem to involve some nontrivial combinatorial optimization to build the minimal tree, but I couldn't see how to factor the left-to-right order of the rules into a hardness proof. In fact, I couldn't think of any NP-complete problem that had such a left-right ordering constraint. After all, if a given set of rules contained a character position in common to all the rules, this character position must be probed first in any minimum-size tree. Since the rules were ordered, each node in the subtree must represent the root of a run of consecutive rules. Thus there were only $\binom{n}{2}$ possible nodes to choose from for this tree....

Bingo! That settled it.

The next day I went back to the professor and told him. "I can't prove that your problem is NP-complete. But how would you feel about an efficient dynamic programming algorithm to find the best trie!" It was a pleasure watching his frown change to a smile as the realization took hold. An efficient algorithm to compute what he needed was infinitely better than a proof saying you couldn't do it!

My recurrence looked something like this. Suppose that we are given n ordered rule heads $s_1, \ldots, s_n$, each with m arguments. Probing at the pth position, $1 \leq p \leq m$, partitioned the rule heads into runs $R_1, \ldots, R_r$, where each rule in a given run $R_x = s_i, \ldots, s_j$ had the same character value of $s_i[p]$. The rules in each run must be consecutive, so there are only $\binom{n}{2}$ possible runs to worry about. The cost of probing at position p is the cost of finishing the trees formed by each created run, plus one edge per tree to link it to probe p:

$$C[i,j] = \min_{p=1}^{m} \sum_{k=1}^{r} (C[i_k, j_k] + 1)$$

A graduate student immediately set to work implementing this algorithm to compare with their heuristic. On many inputs, the optimal and greedy algorithms constructed the exact same trie. However, for some examples, dynamic programming gave a 20% performance improvement over greedy—i.e. , 20% better than very, very well in practice. The run time spent in doing the dynamic programming was a bit larger than with greedy, but in compiler optimization you are always happy to trade off a little extra compilation time for better execution time in the performance of your program. Is a 20% improvement worth this effort? That depends upon the situation. How useful would you find a 20% increase in your salary?

The fact that the rules had to remain ordered was the crucial property that we exploited in the dynamic programming solution. Indeed, without it I was able to prove that the problem *was* NP-complete, something we put in the paper to make it complete.

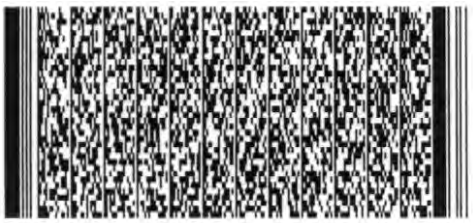

Figure 8.13: A two-dimensional bar-code label of the Gettysburg Address using PDF-417.

Take-Home Lesson: The global optimum (found, for example, using dynamic programming) is often noticeably better than the solution found by typical heuristics. How important this improvement is depends on your application, but it can never hurt.

8.9 War Story: Text Compression for Bar Codes

Ynjiun waved his laser wand over the torn and crumpled fragments of a bar code label. The system hesitated for a few seconds, then responded with a pleasant *blip* sound. He smiled at me in triumph. "Virtually indestructible."

I was visiting the research laboratories of Symbol Technologies, the world's leading manufacturer of bar code scanning equipment. Next time you are in the checkout line at a grocery store, check to see what type of scanning equipment they are using. Likely it will say Symbol on the housing.

Although we take bar codes for granted, there is a surprising amount of technology behind them. Bar codes exist because conventional optical character recognition (OCR) systems are not sufficiently reliable for inventory operations. The bar code symbology familiar to us on each box of cereal or pack of gum encodes a ten-digit number with enough error correction that it is virtually impossible to scan the wrong number, even if the can is upside-down or dented. Occasionally, the cashier won't be able to get a label to scan at all, but once you hear that *blip* you know it was read correctly.

The ten-digit capacity of conventional bar code labels provides room enough only to store a single ID number in a label. Thus any application of supermarket bar codes must have a database mapping 11141-47011 to a particular size and brand of soy sauce. The holy grail of the bar code world has long been the development of higher-capacity bar code symbologies that can store entire documents, yet still be read reliably.

"PDF-417 is our new, two-dimensional bar code symbology," Ynjiun explained. A sample label is shown in Figure 8.13.

"How much data can you fit in a typical one-inch square label?" I asked him.

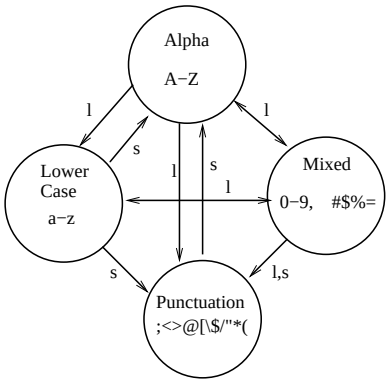

Figure 8.14: Mode switching in PDF-417

"It depends upon the level of error correction we use, but about 1,000 bytes. That's enough for a small text file or image," he said.

"Interesting. You will probably want to use some data compression technique to maximize the amount of text you can store in a label." See Section 18.5 (page 637) for a discussion of standard data compression algorithms.

"We do incorporate a data compaction method," he explained. "We think we understand the different types of files our customers will want to make labels for. Some files will be all in uppercase letters, while others will use mixed-case letters and numbers. We provide four different text modes in our code, each with a different subset of alphanumeric characters available. We can describe each character using only five bits as long as we stay within a mode. To switch modes, we issue a mode switch command first (taking an extra five bits) and then the new character code."

"I see. So you designed the mode character sets to minimize the number of mode switch operations on typical text files." The modes are illustrated in Figure 8.14.

"Right. We put all the digits in one mode and all the punctuation characters in another. We also included both mode *shift* and mode *latch* commands. In a mode shift, we switch into a new mode just for the next character, say to produce a punctuation mark. This way, we don't pay a cost for returning back to text mode after a period. Of course, we can also latch permanently into a different mode if we will be using a run of several characters from there."

"Wow!" I said. "With all of this mode switching going on, there must be many different ways to encode any given text as a label. How do you find the smallest of such encoding."

"We use a greedy algorithm. We look a few characters ahead and then decide which mode we would be best off in. It works fairly well."

I pressed him on this. "How do you know it works fairly well? There might be significantly better encodings that you are simply not finding."

"I guess I don't know. But it's probably NP-complete to find the optimal coding." Ynjiun's voice trailed off. "Isn't it?"

I started to think. Every encoding started in a given mode and consisted of a sequence of intermixed character codes and mode shift/latch operations. At any given position in the text, we could output the next character code (if it was available in our current mode) or decide to shift. As we moved from left to right through the text, our current state would be completely reflected by our current character position and current mode state. For a given position/mode pair, we would have been interested in the cheapest way of getting there, over all possible encodings getting to this point....

My eyes lit up so bright they cast shadows on the walls.

"The optimal encoding for any given text in PDF-417 can be found using dynamic programming. For each possible mode $1 \leq m \leq 4$, and each character position $1 \leq i \leq n$, we will maintain the cheapest encoding found of the first i characters ending in mode m. Our next move from each mode/position is either match, shift, or latch, so there are only a few possible operations to consider."

Basically,

$$M[i,j] = \min_{1 \leq m \leq 4} (M[i-1,m] + c(S_i, m, j))$$

where $c(S_i, m, j)$ is the cost of encoding character S_i and switching from mode m to mode j. The cheapest possible encoding results from tracing back from $M[n,m]$, where m is the value of i that minimizes $\min_{1 \leq i \leq 4} M[n,i]$. Each of the $4n$ cells can be filled in constant time, so it takes time linear in the length of the string to find the optimal encoding.

Ynjiun was skeptical, but he encouraged us to implement an optimal encoder. A few complications arose due to weirdnesses of PDF-417 mode switching, but my student Yaw-Ling Lin rose to the challenge. Symbol compared our encoder to theirs on 13,000 labels and concluded that dynamic programming lead to an 8% tighter encoding on average. This was significant, because no one wants to waste 8% of their potential storage capacity, particularly in an environment where the capacity is only a few hundred bytes. For certain applications, this 8% margin permitted one bar code label to suffice where previously two had been required. Of course, an 8% *average* improvement meant that it did much better than that on certain labels. While our encoder took slightly longer to run than the greedy encoder, this was not significant, since the bottleneck would be the time needed to print the label anyway.

Our observed impact of replacing a heuristic solution with the global optimum is probably typical of most applications. Unless you really botch your heuristic, you are probably going to get a decent solution. Replacing it with an optimal result, however, usually gives a small but nontrivial improvement, which can have pleasing consequences for your application.

Chapter Notes

Bellman [Bel58] is credited with developing the technique of dynamic programming. The edit distance algorithm is originally due to Wagner and Fischer [WF74]. A faster algorithm for the book partition problem appears in [KMS97].

The computational complexity of finding the minimum weight triangulation of disconnected point sets (as opposed to polygons) was a longstanding open problem that finally fell to Mulzer and Rote [MR06].

Techniques such as dynamic programming and backtracking searches can be used to generate worst-case efficient (although still non-polynomial) algorithms for many NP-complete problems. See Woeginger [Woe03] for a nice survey of such techniques.

The morphing system that was the subject of the war story in Section 8.4 (page 291) is described in [HWK94]. See our paper [DRR+95] for more on the Prolog trie minimization problem, subject of the war story of Section 8.8 (page 304). Two-dimensional bar codes, subject of the war story in Section 8.9 (page 307), were developed largely through the efforts of Theo Pavlidis and Ynjiun Wang at Stony Brook [PSW92].

The dynamic programming algorithm presented for parsing is known as the *CKY* algorithm after its three independent inventors (Cocke, Kasami, and Younger) [You67]. The generalization of parsing to edit distance is due to Aho and Peterson [AP72].

8.10 Exercises

Edit Distance

8-1. *[3]* Typists often make transposition errors exchanging neighboring characters, such as typing "setve" when you mean "steve." This requires two substitutions to fix under the conventional definition of edit distance.

Incorporate a swap operation into our edit distance function, so that such neighboring transposition errors can be fixed at the cost of one operation.

8-2. *[4]* Suppose you are given three strings of characters: X, Y, and Z, where $|X| = n$, $|Y| = m$, and $|Z| = n + m$. Z is said to be a *shuffle* of X and Y iff Z can be formed by interleaving the characters from X and Y in a way that maintains the left-to-right ordering of the characters from each string.

(a) Show that *cchocohilaptes* is a shuffle of *chocolate* and *chips*, but *chocochilatspe* is not.

(b) Give an efficient dynamic-programming algorithm that determines whether Z is a shuffle of X and Y. Hint: the values of the dynamic programming matrix you construct should be Boolean, not numeric.

8-3. *[4]* The longest common *substring* (not subsequence) of two strings X and Y is the longest string that appears as a run of consecutive letters in both strings. For example, the longest common substring of *photograph* and *tomography* is *ograph*.

(a) Let $n = |X|$ and $m = |Y|$. Give a $\Theta(nm)$ dynamic programming algorithm for longest common substring based on the longest common subsequence/edit distance algorithm.

(b) Give a simpler $\Theta(nm)$ algorithm that does not rely on dynamic programming.

8-4. *[6]* The *longest common subsequence (LCS)* of two sequences T and P is the longest sequence L such that L is a subsequence of both T and P. The *shortest common supersequence (SCS)* of T and P is the smallest sequence L such that both T and P are a subsequence of L.

(a) Give efficient algorithms to find the LCS and SCS of two given sequences.

(b) Let $d(T, P)$ be the minimum edit distance between T and P when no substitutions are allowed (i.e., the only changes are character insertion and deletion). Prove that $d(T, P) = |SCS(T, P)| - |LCS(T, P)|$ where $|SCS(T, P)|$ ($|LCS(T, P)|$) is the size of the shortest SCS (longest LCS) of T and P.

Greedy Algorithms

8-5. *[4]* Let $P_1, P_2, \ldots, P_n$ be n programs to be stored on a disk with capacity D megabytes. Program P_i requires s_i megabytes of storage. We cannot store them all because $D < \sum_{i=1}^{n} s_i$

(a) Does a greedy algorithm that selects programs in order of nondecreasing s_i maximize the number of programs held on the disk? Prove or give a counterexample.

(b) Does a greedy algorithm that selects programs in order of nonincreasing order s_i use as much of the capacity of the disk as possible? Prove or give a counterexample.

8-6. *[5]* Coins in the United States are minted with denominations of 1, 5, 10, 25, and 50 cents. Now consider a country whose coins are minted with denominations of $\{d_1, \ldots, d_k\}$ units. We seek an algorithm to make change of n units using the minimum number of coins for this country.

(a) The greedy algorithm repeatedly selects the biggest coin no bigger than the amount to be changed and repeats until it is zero. Show that the greedy algorithm does not always use the minimum number of coins in a country whose denominations are $\{1, 6, 10\}$.

(b) Give an efficient algorithm that correctly determines the minimum number of coins needed to make change of n units using denominations $\{d_1, \ldots, d_k\}$. Analyze its running time.

8-7. *[5]* In the United States, coins are minted with denominations of 1, 5, 10, 25, and 50 cents. Now consider a country whose coins are minted with denominations of $\{d_1, \ldots, d_k\}$ units. We want to count how many distinct ways $C(n)$ there are to make change of n units. For example, in a country whose denominations are $\{1, 6, 10\}$, $C(5) = 1$, $C(6)$ to $C(9) = 2$, $C(10) = 3$, and $C(12) = 4$.

(a) How many ways are there to make change of 20 units from $\{1, 6, 10\}$?

(b) Give an efficient algorithm to compute $C(n)$, and analyze its complexity. (Hint: think in terms of computing $C(n, d)$, the number of ways to make change of n units with highest denomination d. Be careful to avoid overcounting.)

8-8. *[6]* In the *single-processor scheduling problem*, we are given a set of n jobs J. Each job i has a processing time t_i, and a deadline d_i. A feasible schedule is a permutation of the jobs such that when the jobs are performed in that order, every job is finished before its deadline. The greedy algorithm for single-processor scheduling selects the job with the earliest deadline first.

Show that if a feasible schedule exists, then the schedule produced by this greedy algorithm is feasible.

Number Problems

8-9. *[6]* The *knapsack problem* is as follows: given a set of integers $S = \{s_1, s_2, \ldots, s_n\}$, and a given target number T, find a subset of S that adds up exactly to T. For example, within $S = \{1, 2, 5, 9, 10\}$ there is a subset that adds up to $T = 22$ but not $T = 23$.

Give a correct programming algorithm for knapsack that runs in $O(nT)$ time.

8-10. *[6]* The *integer partition* takes a set of positive integers $S = s_1, \ldots, s_n$ and asks if there is a subset $I \in S$ such that

$$\sum_{i \in I} s_i = \sum_{i \notin I} s_i$$

Let $\sum_{i \in S} s_i = M$. Give an $O(nM)$ dynamic programming algorithm to solve the integer partition problem.

8-11. *[5]* Assume that there are n numbers (some possibly negative) on a circle, and we wish to find the maximum contiguous sum along an arc of the circle. Give an efficient algorithm for solving this problem.

8-12. *[5]* A certain string processing language allows the programmer to break a string into two pieces. It costs n units of time to break a string of n characters into two pieces, since this involves copying the old string. A programmer wants to break a string into many pieces, and the order in which the breaks are made can affect the total amount of time used. For example, suppose we wish to break a 20-character string after characters 3, 8, and 10. If the breaks are made in left-right order, then the first break costs 20 units of time, the second break costs 17 units of time, and the third break costs 12 units of time, for a total of 49 steps. If the breaks are made in right-left order, the first break costs 20 units of time, the second break costs 10 units of time, and the third break costs 8 units of time, for a total of only 38 steps.

Give a dynamic programming algorithm that takes a list of character positions after which to break and determines the cheapest break cost in $O(n^3)$ time.

8-13. *[5]* Consider the following data compression technique. We have a table of m text strings, each at most k in length. We want to encode a data string D of length n using as few text strings as possible. For example, if our table contains *(a,ba,abab,b)* and the data string is *bababbaababa*, the best way to encode it is *(b,abab,ba,abab,a)*—a total of five code words. Give an $O(nmk)$ algorithm to find the length of the best

encoding. You may assume that every string has at least one encoding in terms of the table.

8-14. *[5]* The traditional world chess championship is a match of 24 games. The current champion retains the title in case the match is a tie. Each game ends in a win, loss, or draw (tie) where wins count as 1, losses as 0, and draws as 1/2. The players take turns playing white and black. White has an advantage, because he moves first. The champion plays white in the first game. He has probabilities w_{w}, w_{d}, and w_{l} of winning, drawing, and losing playing white, and has probabilities b_{w}, b_{d}, and b_{l} of winning, drawing, and losing playing black.

(a) Write a recurrence for the probability that the champion retains the title. Assume that there are g games left to play in the match and that the champion needs to win i games (which may end in a 1/2).

(b) Based on your recurrence, give a dynamic programming to calculate the champion's probability of retaining the title.

(c) Analyze its running time for an n game match.

8-15. *[8]* Eggs break when dropped from great enough height. Specifically, there must be a floor f in any sufficiently tall building such that an egg dropped from the fth floor breaks, but one dropped from the $(f-1)$st floor will not. If the egg always breaks, then $f = 1$. If the egg never breaks, then $f = n + 1$.

You seek to find the critical floor f using an n-story building. The only operation you can perform is to drop an egg off some floor and see what happens. You start out with k eggs, and seek to drop eggs as few times as possible. Broken eggs cannot be reused. Let $E(k, n)$ be the minimum number of egg droppings that will always suffice.

(a) Show that $E(1, n) = n$.

(b) Show that $E(k, n) = \Theta(n^{\frac{1}{k}})$.

(c) Find a recurrence for $E(k, n)$. What is the running time of the dynamic program to find $E(k, n)$?

Graph Problems

8-16. *[4]* Consider a city whose streets are defined by an $X \times Y$ grid. We are interested in walking from the upper left-hand corner of the grid to the lower right-hand corner.

Unfortunately, the city has bad neighborhoods, whose intersections we do not want to walk in. We are given an $X \times Y$ matrix BAD, where *BAD[i,j] = "yes"* if and only if the intersection between streets i and j is in a neighborhood to avoid.

(a) Give an example of the contents of BAD such that there is no path across the grid avoiding bad neighborhoods.

(b) Give an $O(XY)$ algorithm to find a path across the grid that avoids bad neighborhoods.

(c) Give an $O(XY)$ algorithm to find the *shortest* path across the grid that avoids bad neighborhoods. You may assume that all blocks are of equal length. For partial credit, give an $O(X^2Y^2)$ algorithm.

8-17. *[5]* Consider the same situation as the previous problem. We have a city whose streets are defined by an $X \times Y$ grid. We are interested in walking from the upper left-hand corner of the grid to the lower right-hand corner. We are given an $X \times Y$ matrix BAD, where $BAD[i,j]$ = *"yes"* if and only if the intersection between streets i and j is somewhere we want to avoid.

If there were no bad neighborhoods to contend with, the shortest path across the grid would have length $(X-1)+(Y-1)$ blocks, and indeed there would be many such paths across the grid. Each path would consist of only rightward and downward moves.

Give an algorithm that takes the array BAD and returns the *number* of safe paths of length $X+Y-2$. For full credit, your algorithm must run in $O(XY)$.

Design Problems

8-18. *[4]* Consider the problem of storing n books on shelves in a library. The order of the books is fixed by the cataloging system and so cannot be rearranged. Therefore, we can speak of a book b_i, where $1 \leq i \leq n$, that has a thickness t_i and height h_i. The length of each bookshelf at this library is L.

Suppose all the books have the same height h (i.e. , $h = h_i = h_j$ for all i, j) and the shelves are all separated by a distance of greater than h, so any book fits on any shelf. The greedy algorithm would fill the first shelf with as many books as we can until we get the smallest i such that b_i does not fit, and then repeat with subsequent shelves. Show that the greedy algorithm always finds the optimal shelf placement, and analyze its time complexity.

8-19. *[6]* This is a generalization of the previous problem. Now consider the case where the height of the books is not constant, but we have the freedom to adjust the height of each shelf to that of the tallest book on the shelf. Thus the cost of a particular layout is the sum of the heights of the largest book on each shelf.

- Give an example to show that the greedy algorithm of stuffing each shelf as full as possible does not always give the minimum overall height.
- Give an algorithm for this problem, and analyze its time complexity. Hint: use dynamic programming.

8-20. *[5]* We wish to compute the laziest way to dial given n-digit number on a standard push-button telephone using two fingers. We assume that the two fingers start out on the * and # keys, and that the effort required to move a finger from one button to another is proportional to the Euclidean distance between them. Design an algorithm that computes the method of dialing that involves moving your fingers the smallest amount of total distance, where k is the number of distinct keys on the keypad ($k = 16$ for standard telephones). Try to use $O(nk^3)$ time.

8-21. *[6]* Given an array of n real numbers, consider the problem of finding the maximum sum in any contiguous subvector of the input. For example, in the array

$$\{31, -41, 59, 26, -53, 58, 97, -93, -23, 84\}$$

the maximum is achieved by summing the third through seventh elements, where $59+26+(-53)+58+97 = 187$. When all numbers are positive, the entire array is the answer, while when all numbers are negative, the empty array maximizes the total at 0.

- Give a simple, clear, and correct $\Theta(n^2)$-time algorithm to find the maximum contiguous subvector.
- Now give a $\Theta(n)$-time dynamic programming algorithm for this problem. To get partial credit, you may instead give a *correct* $O(n \log n)$ divide-and-conquer algorithm.

8-22. *[7]* Consider the problem of examining a string $x = x_1 x_2 \ldots x_n$ from an alphabet of k symbols, and a multiplication table over this alphabet. Decide whether or not it is possible to parenthesize x in such a way that the value of the resulting expression is a, where a belongs to the alphabet. The multiplication table is neither commutative or associative, so the order of multiplication matters.

	a	b	c
a	a	c	c
b	a	a	b
c	c	c	c

For example, consider the above multiplication table and the string *bbbba*. Parenthesizing it $(b(bb))(ba)$ gives a, but $((((bb)b)b)a)$ gives c.
Give an algorithm, with time polynomial in n and k, to decide whether such a parenthesization exists for a given string, multiplication table, and goal element.

8-23. *[6]* Let α and β be constants. Assume that it costs α to go left in a tree, and β to go right. Devise an algorithm that builds a tree with optimal worst case cost, given keys $k_1, \ldots, k_n$ and the probabilities that each will be searched $p_1, \ldots, p_n$.

Interview Problems

8-24. *[5]* Given a set of coin denominators, find the minimum number of coins to make a certain amount of change.

8-25. *[5]* You are given an array of n numbers, each of which may be positive, negative, or zero. Give an efficient algorithm to identify the index positions i and j to the maximum sum of the ith through jth numbers.

8-26. *[7]* Observe that when you cut a character out of a magazine, the character on the reverse side of the page is also removed. Give an algorithm to determine whether you can generate a given string by pasting cutouts from a given magazine. Assume that you are given a function that will identify the character and its position on the reverse side of the page for any given character position.

Programming Challenges

These programming challenge problems with robot judging are available at *http://www.programming-challenges.com* or *http://online-judge.uva.es*.

8-1. "Is Bigger Smarter?" – Programming Challenges 111101, UVA Judge 10131.

8-2. "Weights and Measures" – Programming Challenges 111103, UVA Judge 10154.

8-3. "Unidirectional TSP" – Programming Challenges 111104, UVA Judge 116.

8-4. "Cutting Sticks" – Programming Challenges 111105, UVA Judge 10003.

8-5. "Ferry Loading" – Programming Challenges 111106, UVA Judge 10261.

9

Intractable Problems and Approximation Algorithms

We now introduce techniques for proving that *no* efficient algorithm exists for a given problem. The practical reader is probably squirming at the notion of proving anything, and will be particularly alarmed at the idea of investing time to prove that something does not exist. Why are you better off knowing that something you don't know how to do in fact can't be done at all?

The truth is that the theory of NP-completeness is an immensely useful tool for the algorithm designer, even though all it provides are negative results. The theory of NP-completeness enables the algorithm designer to focus her efforts more productively, by revealing that the search for an efficient algorithm for this particular problem is doomed to failure. When one *fails* to show a problem is hard, that suggests there may well be an efficient algorithm to solve it. Two of the war stories in this book described happy results springing from bogus claims of hardness.

The theory of NP-completeness also enables us to identify what properties make a particular problem hard. This provides direction for us to model it in different ways or exploit more benevolent characteristics of the problem. Developing a sense for which problems are hard is an important skill for algorithm designers, and only comes from hands-on experience with proving hardness.

The fundamental concept we will use is that of *reductions* between pairs of problems, showing that the problems are really equivalent. We illustrate this idea through a series of reductions, each of which either yields an efficient algorithm or an argument that no such algorithm can exist. We also provide brief introductions to (1) the complexity-theoretic aspects of NP-completeness, one of the most fundamental notions in Computer Science, and (2) the theory of approximation algorithms, which leads to heuristics that probably return something *close* to the optimal solution.

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9.1 Problems and Reductions

We have encountered several problems in this book for which we couldn't find any efficient algorithm. The theory of NP-completeness provides the tools needed to show that all these problems are on some level really the same problem.

The key idea to demonstrating the hardness of a problem is that of a *reduction*, or translation, between two problems. The following allegory of NP-completeness may help explain the idea. A bunch of kids take turns fighting each other in the schoolyard to prove how "tough" they are. Adam beats up Bill, who then beats up Chuck. So who if any among them is "tough?" The truth is that there is no way to know without an external standard. If I told you that Chuck was in fact Chuck Norris, certified tough guy, you have to be impressed—both Adam and Bill are at least as tough as he is. On the other hand, suppose I tell you it is a kindergarten school yard. No one would call me tough, but even I can take out Adam. This proves that none of the three of them should be called be tough. In this allegory, each fight represents a reduction. Chuck Norris takes on the role of satisfiability—a certifiably hard problem. The part of an inefficient algorithm with a possible shot at redemption is played by me.

Reductions are operations that convert one problem into another. To describe them, we must be somewhat rigorous in our definitions. An algorithmic *problem* is a general question, with parameters for input and conditions on what constitutes a satisfactory answer or solution. An *instance* is a problem with the input parameters specified. The difference can be made clear by an example:

Problem: The Traveling Salesman Problem (TSP)
Input: A weighted graph G.
Output: Which tour $\{v_1, v_2, ..., v_n\}$ minimizes $\sum_{i=1}^{n-1} d[v_i, v_{i+1}] + d[v_n, v_1]$?

Any weighted graph defines an instance of TSP. Each particular *problem* has at least one minimum cost tour. The general traveling salesman *instance* asks for an algorithm to find the optimal tour for all possible instances.

9.1.1 The Key Idea

Now consider two algorithmic problems, called *Bandersnatch* and *Bo-billy*. Suppose that I gave you the following reduction/algorithm to solve the *Bandersnatch* problem:

Bandersnatch(G)
    Translate the input G to an instance Y of the Bo-billy problem.
    Call the subroutine Bo-billy on Y to solve this instance.
    Return the answer of Bo-billy(Y) as the answer to Bandersnatch(G).

This algorithm will *correctly* solve the Bandersnatch problem provided that the translation to Bo-billy always preserves the correctness of the answer. In other words, the translation has the property that for any instance of G,

$$\text{Bandersnatch}(G) = \text{Bo-billy}(Y)$$

A translation of instances from one type of problem to instances of another such that the answers are preserved is what is meant by a *reduction*.

Now suppose this reduction translates G to Y in $O(P(n))$ time. There are two possible implications:

- *If* my Bo-billy subroutine ran in $O(P'(n))$, this means I could solve the Bandersnatch problem in $O(P(n) + P'(n))$ by spending the time to translate the problem and then the time to execute the Bo-Billy subroutine.
- *If* I know that $\Omega(P'(n))$ is a lower bound on computing Bandersnatch, meaning there definitely exists no faster way to solve it, then $\Omega(P'(n) - P(n))$ *must* be a lower bound to compute Bo-billy. Why? If I could solve Bo-billy any faster, then I could violate my lower bound by solving Bandersnatch using the above reduction. This implies that there can be no way to solve Bo-billy any faster than claimed.

This first argument is Steve demonstrating the weakness of the entire schoolyard with a quick right to Adam's chin. The second highlights the Chuck Norris approach we will use to prove that problems are hard. Essentially, this reduction shows that Bo-billy is no easier than Bandersnatch. Therefore, if Bandersnatch is hard this means Bo-billy must also be hard.

We will illustrate this point by giving several problem reductions in this chapter.

> *Take-Home Lesson:* Reductions are a way to show that two problems are essentially identical. A fast algorithm (or the lack of one) for one of the problems implies a fast algorithm (or the lack of one) for the other.

9.1.2 Decision Problems

Reductions translate between problems so that their answers are identical in every problem instance. Problems differ in the *range* or *type* of possible answers. The traveling salesman problem returns a permutation of vertices as the answer, while other types of problems return numbers as answers, perhaps restricted to positive numbers or integers.

The simplest interesting class of problems have answers restricted to true and false. These are called *decision problems*. It proves convenient to reduce/translate answers between decision problems because both only allow true and false as possible answers.

Fortunately, most interesting optimization problems can be phrased as decision problems that capture the essence of the computation. For example, the traveling salesman decision problem could be defined as:

Problem: The Traveling Salesman Decision Problem
Input: A weighted graph G and integer k.
Output: Does there exist a TSP tour with cost $\leq k$?

The decision version captures the heart of the traveling salesman problem, in that if you had a fast algorithm for the decision problem, you could use it to do a binary search with different values of k and quickly hone in on the optimal solution. With a little more cleverness, you could reconstruct the actual tour permutation using a fast solution to the decision problem.

From now on we will generally talk about decision problems, because it proves easier and still captures the power of the theory.

9.2 Reductions for Algorithms

An engineer and an algorist are sitting in a kitchen. The algorist asks the engineer to boil some water, so the engineer gets up, picks up the kettle from the counter top, adds water from the sink, brings it to the burner, turns on the burner, waits for the whistling sound, and turns off the burner. Sometime later, the engineer asks the algorist to boil more water. She gets up, takes the kettle from the burner, moves it over to the counter top, and sits down. "Done." she says, "I have *reduced* the task to a solved problem."

This boiling water reduction illustrates an honorable way to generate new algorithms from old. If we can translate the input for a problem we *want to solve* into input for a problem we *know how to solve*, we can compose the translation and the solution into an algorithm for our problem.

In this section, we look at several reductions that lead to efficient algorithms. To solve problem a, we translate/reduce the a instance to an instance of b, then solve this instance using an efficient algorithm for problem b. The overall running time is the time needed to perform the reduction plus that solve the b instance.

9.2.1 Closest Pair

The *closest pair* problem asks to find the pair of numbers within a set that have the smallest difference between them. We can make it a decision problem by asking if this value is less than some threshold:

Input: A set S of n numbers, and threshold t.
Output: Is there a pair $s_i, s_j \in S$ such that $|s_i - s_j| \leq t$?

The closest pair is a simple application of sorting, since the closest pair must be neighbors after sorting. This gives the following algorithm:

CloseEnoughPair(S,t)
    Sort S.
    Is $\min_{1 \leq i < n} |s_i - s_{i+1}| \leq t$?

There are several things to note about this simple reduction.

1. The decision version captured what is interesting about the problem, meaning it is no easier than finding the actual closest pair.
2. The complexity of this algorithm depends upon the complexity of sorting. Use an $O(n \log n)$ algorithm to sort, and it takes $O(n \log n + n)$ to find the closest pair.
3. This reduction and the fact that there is an $\Omega(n \log n)$ lower bound on sorting *does not* prove that a close-enough pair must take $\Omega(n \log n)$ time in the worst case. Perhaps this is just a slow algorithm for a close-enough pair, and there is a faster one lurking somewhere?
4. On the other hand, *if* we knew that a close-enough pair required $\Omega(n \log n)$ time to solve in the worst case, this reduction would suffice to prove that sorting couldn't be solved any faster than $\Omega(n \log n)$ because that would imply a faster algorithm for a close-enough pair.

9.2.2 Longest Increasing Subsequence

In Chapter 8, we demonstrated how dynamic programming can be used to solve a variety of problems, including string edit distance (Section 8.2 (page 280)) and longest increasing subsequence (Section 8.3 (page 289)). To review,

Problem: Edit Distance
Input: Integer or character sequences S and T; penalty costs for each insertion (c_{ins}), deletion (c_{del}), and substitution (c_{del}).
Output: What is the minimum cost sequence of operations to transform S to T?

Problem: Longest Increasing Subsequence
Input: An integer or character sequence S.
Output: What is the longest sequence of integer positions $\{p_1, \ldots, p_m\}$ such that $p_i < p_{i+1}$ and $S_{p_i} < S_{p_{i+1}}$?

In fact, longest increasing subsequence (LIS) can be solved as a special case of edit distance:

```
Longest Increasing Subsequence(S)
    T = Sort(S)
    c_ins = c_del = 1
    c_sub = ∞
    Return (|S| - EditDistance(S,T,c_ins,c_del,c_del)/2)
```

Why does this work? By constructing the second sequence T as the elements of S sorted in increasing order, we ensure that any common subsequence must be an

increasing subsequence. If we are never allowed to do any substitutions (because $c_{sub} = \infty$), the optimal alignment of two sequences finds the longest common subsequence between them and removes everything else. Thus, transforming $\{3, 1, 2\}$ to $\{1, 2, 3\}$ costs two, namely inserting and deleting the unmatched 3. The length of S minus half this cost gives the length of the LIS.

What are the implications of this reduction? The reduction takes $O(n \log n)$ time. Because edit distance takes time $O(|S| \cdot |T|)$, this gives a quadratic algorithm to find the longest increasing subsequence of S, which is the same complexity as the the algorithm presented in Section 8.3 (page 289). In fact, there exists a faster $O(n \log n)$ algorithm for LIS using clever data structures, while edit distance is known to be quadratic in the worst case. Here, our reduction gives us a simple but not optimal polynomial-time algorithm.

9.2.3 Least Common Multiple

The *least common multiple* and *greatest common divisor* problems arise often in working with integers. We say b *divides* a ($b|a$) if there exists an integer d that $a = bd$. Then:

Problem: Least Common Multiple (lcm)
Input: Two integers x and y.
Output: Return the smallest integer m such that m is a multiple of x and m is also a multiple of y.

Problem: Greatest Common Divisor (gcd)
Input: Two integers x and y.
Output: Return the largest integer d such that d divides x and d divides y.

For example, $lcm(24, 36) = 72$ and $gcd(24, 36) = 12$. Both problems can be solved easily after reducing x and y to their prime factorizations, but no efficient algorithm is known for factoring integers (see Section 13.8 (page 420)). Fortunately, Euclid's algorithm gives an efficient way to solve greatest common divisor without factoring. It is a recursive algorithm that rests on two observations. First,

> if $b|a$, then $gcd(a, b) = b$.

This should be pretty clear. if b divides a, then $a = bk$ for some integer k, and thus $gcd(bk, b) = b$. Second,

> If $a = bt + r$ for integers t and r, then $gcd(a, b) = gcd(b, r)$.

Since $x \cdot y$ is a multiple of both x and y, $lcm(x, y) \leq xy$. The only way that there can be a smaller common multiple is if there is some nontrivial factor shared between x and y. This observation, coupled with Euclid's algorithm, provides an efficient way to compute least common multiple, namely

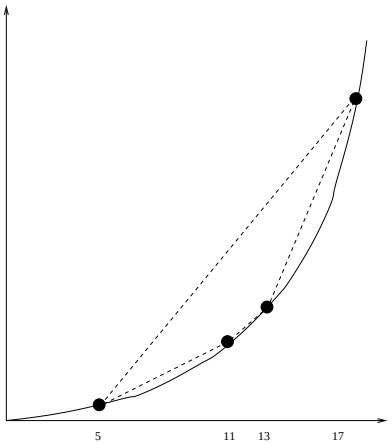

Figure 9.1: Reducing convex hull to sorting by mapping points to a parabola

LeastCommonMultiple(x,y)
Return $(xy/gcd(x,y))$.

This reduction gives us a nice way to reuse Euclid's efforts on another problem.

9.2.4 Convex Hull (*)

Our final example of a reduction from an "easy" problem (i.e. , one that can be solved in polynomial time) goes from finding convex hulls to sorting numbers. A polygon is *convex* if the straight line segment drawn between any two points inside the polygon P must lie completely within the polygon. This is the case when P contains no notches or *concavities*, so convex polygons are nicely shaped. The convex hull provides a very useful way to provide structure to a point set. Applications are presented in Section 17.2 (page 568).

Problem: Convex Hull
Input: A set S of n points in the plane.
Output: Find the smallest convex polygon containing all the points of S.

We now show how to transform from sorting to convex hull. This means we must translate each number to a point. We do so by mapping x to (x, x^2). Why? It means each integer is mapped to a point on the parabola $y = x^2$. Since this parabola is convex, every point must be on the convex hull. Furthermore, since neighboring points on the convex hull have neighboring x values, the convex hull returns the points sorted by the x-coordinate—i.e., the original numbers. Creating and reading off the points takes $O(n)$ time:

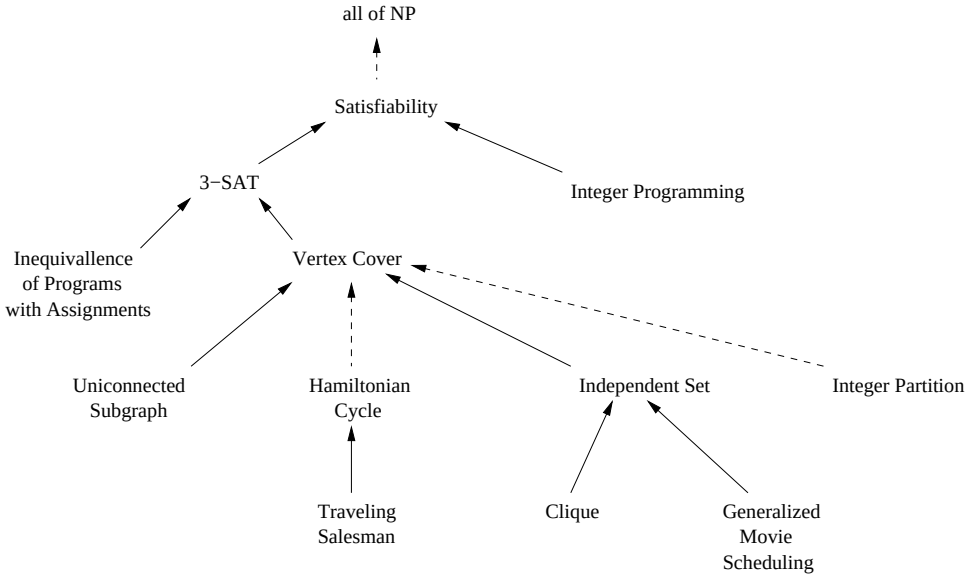

Figure 9.2: A portion of the reduction tree for NP-complete problems. Solid lines denote the reductions presented in this chapter

---

Sort(S)
    For each $i \in S$, create point (i, i^2).
    Call subroutine convex-hull on this point set.
    From the leftmost point in the hull,
        read off the points from left to right.

What does this mean? Recall the sorting lower bound of $\Omega(n \lg n)$. If we could compute convex hull in better than $n \lg n$, this reduction implies that we could sort faster than $\Omega(n \lg n)$, which violates our lower bound. Thus, convex hull must take $\Omega(n \lg n)$ as well! Observe that any $O(n \lg n)$ convex hull algorithm also gives us a complicated but correct $O(n \lg n)$ sorting algorithm as well.

9.3 Elementary Hardness Reductions

The reductions in the previous section demonstrate transformations between pairs of problems for which efficient algorithms exist. However, we are mainly concerned with using reductions to prove hardness, by showing that a fast algorithm for *Bandersnatch* would imply one that cannot exist for *Bo-billy*.

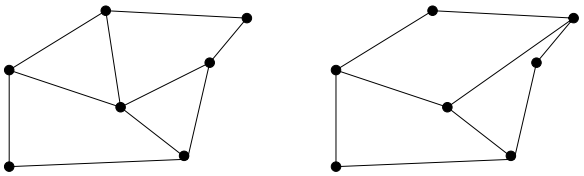

Figure 9.3: Graphs with (l) and without (r) Hamiltonian cycles

For now, I want you to trust me when I say that *Hamiltonian cycle* and *vertex cover* are hard problems. The entire picture (presented in Figure 9.2) will become clear by the end of the chapter.

9.3.1 Hamiltonian Cycle

The Hamiltonian cycle problem is one of the most famous in graph theory. It seeks a tour that visits each vertex of a given graph exactly once. It has a long history and many applications, as discussed in Section 16.5. Formally, it is defined as:

Problem: Hamiltonian Cycle
Input: An unweighted graph G.
Output: Does there exist a simple tour that visits each vertex of G without repetition?

Hamiltonian cycle has some obvious similarity to the traveling salesman problem. Both problems seek a tour that visits each vertex exactly once. There are also differences between the two problems. TSP works on weighted graphs, while Hamiltonian cycle works on unweighted graphs. The following reduction from Hamiltonian cycle to traveling salesman shows that the similarities are greater than the differences:

```
HamiltonianCycle(G = (V, E))
    Construct a complete weighted graph G' = (V', E') where V' = V.
    n = |V|
    for i = 1 to n do
        for j = 1 to n do
            if (i, j) ∈ E then w(i, j) = 1 else w(i, j) = 2
    Return the answer to Traveling-Salesman-Decision-Problem(G', n).
```

The actual reduction is quite simple, with the translation from unweighted to weighted graph easily performed in $O(n^2)$ time. Further, this translation is designed to ensure that the answers of the two problems will be identical. If the graph G has a Hamiltonian cycle $\{v_1, \ldots, v_n\}$, then this exact same tour will correspond to n edges in E', each with weight 1. This gives a TSP tour in G' of weight exactly

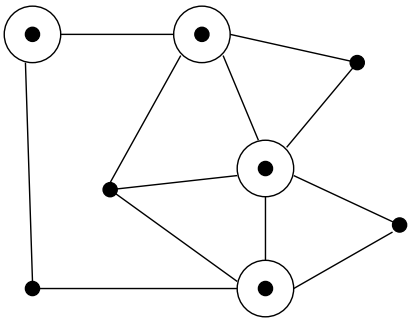

Figure 9.4: Circled vertices form a vertex cover, and the others form an independent set

n. If G does not have a Hamiltonian cycle, then there can be no such TSP tour in G' because the only way to get a tour of cost n in G would be to use only edges of weight 1, which implies a Hamiltonian cycle in G.

This reduction is both efficient and truth preserving. A fast algorithm for TSP would imply a fast algorithm for Hamiltonian cycle, while a hardness proof for Hamiltonian cycle would imply that TSP is hard. Since the latter is the case, this reduction shows that TSP is hard, at least as hard as the Hamiltonian cycle.

9.3.2 Independent Set and Vertex Cover

The vertex cover problem, discussed more thoroughly in Section 16.3 (page 530), asks for a small set of vertices that contacts each edge in a graph. More formally:

Problem: Vertex Cover
Input: A graph $G = (V, E)$ and integer $k \leq |V|$.
Output: Is there a subset S of at most k vertices such that every $e \in E$ contains at least one vertex in S?

It is trivial to find *a* vertex cover of a graph, namely the cover that consists of all the vertices. More tricky is to cover the edges using as small a set of vertices as possible. For the graph in Figure 9.4, four of the eight vertices are sufficient to cover.

A set of vertices S of graph G is *independent* if there are no edges (x, y) where both $x \in S$ and $y \in S$. This means there are no edges between any two vertices in independent set. As discussed in Section 16.2 (page 528), independent set arises in facility location problems. The maximum independent set decision problem is formally defined:

Problem: Independent Set
Input: A graph G and integer $k \leq |V|$.
Output: Does there exist an independent set of k vertices in G?

Both vertex cover and independent set are problems that revolve around finding special subsets of vertices: the first with representatives of every edge, the second with no edges. If S is the vertex cover of G, the remaining vertices $S - V$ must form an independent set, for if an edge had both vertices in $S - V$, then S could not have been a vertex cover. This gives us a reduction between the two problems:

VertexCover(G, k)
    $G' = G$
    $k' = |V| - k$
    Return the answer to IndependentSet(G', k')

Again, a simple reduction shows that the two problems are identical. Notice how this translation occurs without any knowledge of the answer. We transform the *input*, not the solution. This reduction shows that the hardness of vertex cover implies that independent set must also be hard. It is easy to reverse the roles of the two problems in this particular reduction, thus proving that both problems are equally hard.

Stop and Think: Hardness of General Movie Scheduling

Problem: Prove that the *general* movie scheduling problem is NP-complete, with a reduction from independent set.

Problem: General Movie Scheduling Decision Problem
Input: A set I of n *sets of* intervals on the line, integer k.
Output: Can a subset of at least k mutually nonoverlapping interval *sets* which can be selected from I?

Solution: Recall the movie scheduling problem, discussed in Section 1.2 (page 9). Each possible movie project came with a single time interval during which filming took place. We sought the largest possible subset of movie projects such that no two conflicting projects (i.e. , both requiring the actor at the same time) were selected.

The general problem allows movie projects to have discontinuous schedules. For example, Project A running from January-March and May-June does not intersect Project B running in April and August, but *does* collide with Project C running from June-July.

If we are going to prove general movie scheduling hard from independent set, what is Bandersnatch and what is Bo-billy? We need to show how to translate *all* independent set problems into instances of movie scheduling—i.e. , sets of disjointed line intervals.

What is the correspondence between the two problems? Both problems involve selecting the largest subsets possible—of vertices and movies, respectively. This

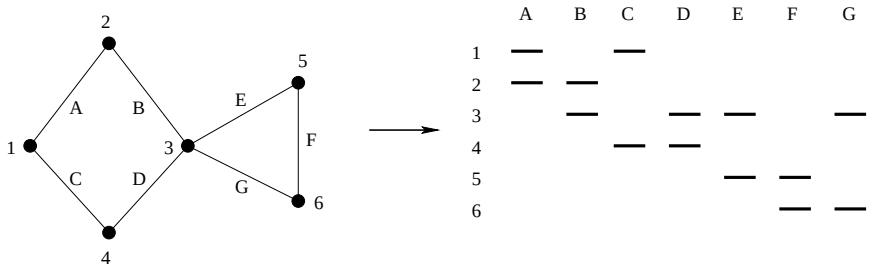

Figure 9.5: Reduction from independent set to generalized movie scheduling, with numbered vertices and lettered edges

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suggests we must translate vertices into movies. Further, both require the selected elements not to interfere, by sharing an edge or overlapping an interval, respectively.

IndependentSet(G, k)
    $I = \emptyset$
    For the ith edge (x, y), $1 \leq i \leq m$
        Add interval $[i, i + 0.5]$ for movie X to I
        Add interval $[i, i + 0.5]$ for movie y to I
    Return the answer to GeneralMovieScheduling(I, k)

My construction is as follows. Create an interval on the line for each of the m edges of the graph. The movie associated with each vertex will contain the intervals for the edges adjacent with it, as shown in Figure 9.5.

Each pair of vertices sharing an edge (forbidden to be in independent set) defines a pair of movies sharing a time interval (forbidden to be in the actor's schedule). Thus, the largest satisfying subsets for both problems are the same, and a fast algorithm for solving general movie scheduling gives us a fast algorithm for solving independent set. Thus, general movie scheduling must be hard as hard as independent set, and hence NP-complete. ∎

9.3.3 Clique

A social clique is a group of mutual friends who all hang around together. A graph-theoretic *clique* is a complete subgraph where each vertex pair has an edge between them. Cliques are the densest possible subgraphs:

Problem: Maximum Clique
Input: A graph $G = (V, E)$ and integer $k \leq |V|$.
Output: Does the graph contain a clique of k vertices; i.e. , is there a subset $S \subset V$, where $|S| \leq k$, such that every pair of vertices in S defines an edge of G?

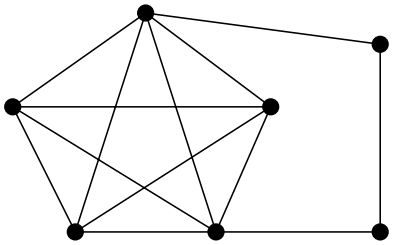


Figure 9.6: A small graph with a five-vertex clique

The graph in Figure 9.6 contains a clique of five vertices. Within the friendship graph, we would expect to see large cliques corresponding to workplaces, neighborhoods, religious organizations, and schools. Applications of cliques are further discussed in Section 16.1 (page 525).

In the independent set problem, we looked for a subset S with no edges between two vertices of S. This contrasts with clique, where we insist that there always be an edge between two vertices. A reduction between these problems follows by reversing the roles of edges and nonedges—an operation known as *complementing* the graph:

IndependentSet(G, k)
    Construct a graph $G' = (V', E')$ where $V' = V$, and
        For all (i, j) not in E, add (i, j) to E'
    Return the answer to Clique(G', k)

These last two reductions provide a chain linking of three different problems. The hardness of clique is implied by the hardness of independent set, which is implied by the hardness of vertex cover. By constructing reductions in a chain, we link together pairs of problems in implications of hardness. Our work is done as soon as all these chains begin with a single problem that is accepted as hard. Satisfiability is the problem that will serve as the first link in this chain.

9.4 Satisfiability

To demonstrate the hardness of all problems using reductions, we must start with a single problem that is absolutely, certifiably, undeniably hard. The mother of all NP-complete problems is a logic problem named *satisfiability*:

Problem: Satisfiability
Input: A set of Boolean variables V and a set of clauses C over V.
Output: Does there exist a satisfying truth assignment for C—i.e. , a way to set the variables $v_1, \ldots, v_n$ true or false so that each clause contains at least one true literal?

This can be made clear with two examples. Suppose that $C = \{\{v_1, \overline{v}_2\}, \{\overline{v}_1, v_2\}\}$ over the Boolean variables $V = \{v_1, v_2\}$. We use $\overline{v}_i$ to denote the complement of the variable v_i, so we get credit for satisfying a particular clause containing v_i if $v_i =$ true, or a clause containing $\overline{v}_i$ if $v_i =$ false. Therefore, satisfying a particular set of clauses involves making a series of n true or false decisions, trying to find the right truth assignment to satisfy all of them.

These example clauses $C = \{\{v_1, \overline{v}_2\}, \{\overline{v}_1, v_2\}\}$ can be satisfied by either setting $v_1 = v_2 =$ true or $v_1 = v_2 =$ false. However, consider the set of clauses $C = \{\{v_1, v_2\}, \{v_1, \overline{v}_2\}, \{\overline{v}_1\}\}$. Here there can be no satisfying assignment, because v_1 must be false to satisfy the third clause, which means that v_2 must be false to satisfy the second clause, which then leaves the first clause unsatisfiable. Although you try, and you try, and you try, and you try, you can't get no satisfaction.

For a combination of social and technical reasons, it is well accepted that satisfiability is a hard problem; one for which no worst-case polynomial-time algorithm exists. Literally every top-notch algorithm expert in the world (and countless lesser lights) have directly or indirectly tried to come up with a fast algorithm to test whether a given set of clauses is satisfiable. All have failed. Furthermore, many strange and impossible-to-believe things in the field of computational complexity have been shown to be true if there exists a fast satisfiability algorithm. Satisfiability is a hard problem, and we should feel comfortable accepting this. See Section 14.10 (page 472) for more on the satisfiability problem and its applications.

9.4.1 3-Satisfiability

Satisfiability's role as the first NP-complete problem implies that the problem is hard to solve in the worst case. But certain special-case instances of the problem are not necessarily so tough. Suppose that each clause contains exactly one literal. We must appropriately set that literal to satisfy such a clause. We can repeat this argument for every clause in the problem instance. Thus only when we have two clauses that directly contradict each other, such as $C = \{\{v_1\}, \{\overline{v}_1\}\}$, will the set not be satisfiable.

Since clause sets with only one literal per clause are easy to satisfy, we are interested in slightly larger classes. How many literals per clause do you need to turn the problem from polynomial to hard? This transition occurs when each clause contains three literals, i.e.

Problem: 3-Satisfiability (3-SAT)
Input: A collection of clauses C where each clause contains exactly 3 literals, over a set of Boolean variables V.
Output: Is there a truth assignment to V such that each clause is satisfied?

Since this is a restricted case of satisfiability, the hardness of 3-SAT implies that satisfiability is hard. The converse isn't true, since the hardness of general satisfiability might depend upon having long clauses. We can show the hardness

of 3-SAT using a reduction that translates every instance of satisfiability into an instance of 3-SAT without changing whether it is satisfiable.

This reduction transforms each clause independently based on its *length*, by adding new clauses and Boolean variables along the way. Suppose clause C_i contained k literals:

- $k = 1$, meaning that $C_i = \{z_1\}$ – We create two new variables v_1, v_2 and four new 3-literal clauses: $\{v_1, v_2, z_1\}$, $\{v_1, \overline{v}_2, z_1\}$, $\{\overline{v}_1, v_2, z_1\}$, $\{\overline{v}_1, \overline{v}_2, z_1\}$. Note that the only way that all four of these clauses can be simultaneously satisfied is if $z_1 =$ true, which also means the original C_i will be satisfied.
- $k = 2$, meaning that $C_i = \{z_1, z_2\}$ – We create one new variable v_1 and two new clauses: $\{v_1, z_1, z_2\}$, $\{\overline{v}_1, z_1, z_2\}$. Again, the only way to satisfy both of these clauses is to have at least one of z_1 and z_2 be true, thus satisfying c_i.
- $k = 3$, meaning that $C_i = \{z_1, z_2, z_3\}$ – We copy C_i into the 3-SAT instance unchanged: $\{z_1, z_2, z_3\}$.
- $k > 3$, meaning that $C_i = \{z_1, z_2, ..., z_n\}$ – We create $n-3$ new variables and $n-2$ new clauses in a chain, where for $2 \leq j \leq n-3$, $C_{i,j} = \{v_{i,j-1}, z_{j+1}, \overline{v}_{i,j}\}$, $C_{i,1} = \{z_1, z_2, \overline{v}_{i,1}\}$, and $C_{i,n-2} = \{v_{i,n-3}, z_{n-1}, z_n\}$.

The most complicated case here is that of the large clauses. If none of the original literals in C_i are true, then there are not enough new variables to be able to satisfy all of the new subclauses. You can satisfy $C_{i,1}$ by setting $v_{i,1} =$ false, but this forces $v_{i,2} =$ false, and so on until finally $C_{i,n-2}$ cannot be satisfied. However, if any single literal $z_i =$ true, then we have $n-3$ free variables and $n-3$ remaining 3-clauses, so we can satisfy each of them.

This transform takes $O(m+n)$ time if there were n clauses and m total literals in the SAT instance. Since any SAT solution also satisfies the 3-SAT instance and any 3-SAT solution describes how to set the variables giving a SAT solution, the transformed problem is equivalent to the original.

Note that a slight modification to this construction would serve to prove that 4-SAT, 5-SAT, or any ($k \geq 3$)-SAT is also NP-complete. However, this construction breaks down if we try to use it for 2-SAT, since there is no way to stuff anything into the chain of clauses. It turns out that a depth-first search on an appropriate graph can be used to give a linear-time algorithm for 2-SAT, as discussed in Section 14.10 (page 472).

9.5 Creative Reductions

Since both satisfiability and 3-SAT are known to be hard, we can use either of them in reductions. Usually 3-SAT is the better choice, because it is simpler to work with. What follows are a pair of more complicated reductions, designed to serve as examples and also increase our repertoire of known hard problems. Many

reductions are quite intricate, because we are essentially programming one problem in the language of a significantly different problem.

One perpetual point of confusion is getting the direction of the reduction right. Recall that we must transform *every* instance of a known NP-complete problem into an instance of the problem we are interested in. If we perform the reduction the other way, all we get is a slow way to solve the problem of interest, by using a subroutine that takes exponential time. This always is confusing at first, for this direction of reduction seems backwards. Make sure you understand the direction of reduction now, and think back to this whenever you get confused.

9.5.1 Integer Programming

As discussed in Section 13.6 (page 411), integer programming is a fundamental combinatorial optimization problem. It is best thought of as linear programming with the variables restricted to take only integer (instead of real) values.

Problem: Integer Programming
Input: A set of integer variables V, a set of inequalities over V, a maximization function $f(V)$, and an integer B.
Output: Does there exist an assignment of integers to V such that all inequalities are true and $f(V) \geq B$?

Consider the following two examples. Suppose

$$v_1 \geq 1, \quad v_2 \geq 0$$

$$v_1 + v_2 \leq 3$$

$$f(v) : 2v_2, \quad B = 3$$

A solution to this would be $v_1 = 1$, $v_2 = 2$. Not all problems have realizable solutions, however. For the following problem:

$$v_1 \geq 1, \quad v_2 \geq 0$$

$$v_1 + v_2 \leq 3$$

$$f(v) : 2v_2, \quad B = 5$$

The maximum possible value of $f(v)$ given the constraints is $2 \times 2 = 4$, so there can be no solution to the associated decision problem.

We show that integer programming is hard using a reduction from 3-SAT. For this particular reduction, general satisfiability would work just as well, although usually 3-SAT makes reductions easier.

In which direction must the reduction go? We want to prove integer programming is hard, and know that 3-SAT is hard. If I could solve 3-SAT using integer

programming and integer programming were easy, this would mean that satisfiability would be easy. Now the direction should be clear; we must translate 3-SAT into integer programming.

What should the translation look like? Every satisfiability instance contains Boolean (true/false) variables and clauses. Every integer programming instance contains integer variables (values restricted to 0,1,2,...) and constraints. A reasonable idea is to make the integer variables correspond to Boolean variables and use constraints to serve the same role as the clauses do in the original problem.

Our translated integer programming problem will have twice as many variables as the SAT instance—one for each variable and one for its complement. For each variable v_i in the set problem, we will add the following constraints:

- We restrict each integer programming variable V_i to values of either 0 or 1, but adding constraints $1 \geq V_i \geq 0$ and $1 \geq \overline{V}_i \geq 0$. Thus coupled with integrality, they correspond to values of true and false.

- We ensure that exactly one of the two integer programming variables associated with a given SAT variable is true, by adding constraints so that $1 \geq V_i + \overline{V}_i \geq 1$.

For each 3-SAT clause $C_i = \{z_1, z_2, z_3\}$, construct a constraint: $V_1 + V_2 + V_3 \geq 1$. To satisfy this constraint, at least one of the literals per clause must be set to 1, thus corresponding to a true literal. Satisfying this constraint is therefore equivalent to satisfying the clause.

The maximization function and bound prove relatively unimportant, since we have already encoded the entire 3-SAT instance. By using $f(v) = V_1$ and $B = 0$, we ensure that they will not interfere with any variable assignment satisfying all the inequalities. Clearly, this reduction can be done in polynomial time. To establish that this reduction preserves the answer, we must verify two things:

- *Any SAT solution gives a solution to the IP problem* – In any SAT solution, a true literal corresponds to a 1 in the integer program, since the clause is satisfied. Therefore, the sum in each clause inequality is ≥ 1.

- *Any IP solution gives a solution to the original SAT problem* – All variables must be set to either 0 or 1 in any solution to this integer programming instance. If $V_i = 1$, then set literal $z_i =$ true. If $V_i = 0$, then set literal $z_i =$ false. This is a legal assignment which must also satisfy all the clauses.

The reduction works both ways, so integer programming must be hard. Notice the following properties, which hold true in general for NP-completeness proofs:

1. This reduction preserved the structure of the problem. It did not *solve* the problem, just put it into a different format.

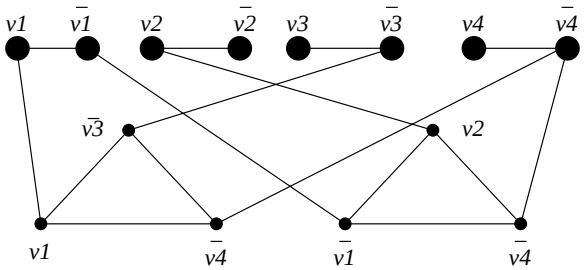


Figure 9.7: Reducing satisfiability instance $\{\{v_1, \bar{v_3}, \bar{v_4}\}, \{\bar{v_1}, v_2, \bar{v_4}\}\}$ to vertex cover

2. The possible IP instances that can result from this transformation are only a small subset of all possible IP instances. However, since some of them are hard, the general problem must be hard.

3. The transformation captures the essence of *why* IP is hard. It has nothing to do with having big coefficients or big ranges of variables, because restricting them to 0/1 is enough. It has nothing to do with having inequalities with large numbers of variables. Integer programming is hard because satisfying a set of constraints is hard. A careful study of the properties needed for a reduction can tell us a lot about the problem.

9.5.2 Vertex Cover

Algorithmic graph theory proves to be a fertile ground for hard problems. The prototypical NP-complete graph problem is vertex cover, previously defined in Section 9.3.2 (page 325) as follows:

Problem: Vertex Cover
Input: A graph $G = (V, E)$ and integer $k \leq |V|$.
Output: Is there a subset S of at most k vertices such that every $e \in E$ has at least one vertex in S?

Demonstrating the hardness of vertex cover proves more difficult than the previous reductions we have seen, because the structure of the two relevant problems is very different. A reduction from 3-satisfiability to vertex cover has to construct a graph G and bound k from the variables and clauses of the satisfiability instance.

First, we translate the variables of the 3-SAT problem. For each Boolean variable v_i, we create two vertices v_i and $\bar{v_i}$ connected by an edge. At least n vertices will be needed to cover all these edges, since no two of the edges will share a vertex.

Second, we translate the clauses of the 3-SAT problem. For each of the c clauses, we create three new vertices, one for each literal in each clause. The three vertices of each clause will be connected so as to form c triangles. At least two vertices per

triangle must be included in any vertex cover of these triangles, for a total of $2c$ cover vertices.

Finally, we will connect these two sets of components together. Each literal in the vertex "gadgets" is connected to vertices in the clause gadgets (triangles) that share the same literal. From a 3-SAT instance with n variables and c clauses, this constructs a graph with $2n + 3c$ vertices. The complete reduction for the 3-SAT problem $\{\{v_1, \bar{v_3}, \bar{v_4}\}, \{\bar{v_1}, v_2, \bar{v_4}\}\}$ is shown in Figure 9.7.

This graph has been designed to have a vertex cover of size $n + 2c$ if and only if the original expression is satisfiable. By the earlier analysis, every vertex cover must have at least $n + 2c$ vertices, since adding the connecting edges to G cannot shrink the size of the vertex cover to less than that of the disconnected vertex and clause gadgets. To show that our reduction is correct, we must demonstrate that:

- *Every satisfying truth assignment gives a vertex cover* – Given a satisfying truth assignment for the clauses, select the n vertices from the vertex gadgets that correspond to true literals to be members of the vertex cover. Since this defines a satisfying truth assignment, a true literal from each clause must cover at least one of the three cross edges connecting each triangle vertex to a vertex gadget. Therefore, by selecting the other two vertices of each clause triangle, we also pick up all remaining cross edges.

- *Every vertex cover gives a satisfying truth assignment* – In any vertex cover C of size $n + 2c$, exactly n of the vertices must belong to the vertex gadgets. Let these first stage vertices define the truth assignment, while the remaining $2c$ cover vertices must be distributed at two per clause gadget. Otherwise a clause gadget edge must go uncovered. These clause gadget vertices can cover only two of the three connecting cross edges per clause. Therefore, if C gives a vertex cover, at least one cross edge per clause must be covered, meaning that the corresponding truth assignment satisfies all clauses.

This proof of the hardness of vertex cover, chained with the clique and independent set reductions of Section 9.3.2 (page 325), gives us a library of hard graph problems that we can use to make future hardness proofs easier.

Take-Home Lesson: A small set of NP-complete problems (3-SAT, vertex cover, integer partition, and Hamiltonian cycle) suffice to prove the hardness of most other hard problems.

9.6 The Art of Proving Hardness

Proving that problems are hard is a skill. But once you get the hang of it, reductions can be surprisingly straightforward and pleasurable to do. Indeed, the dirty little secret of NP-completeness proofs is that they are usually easier to create than explain, in much the same way that it can be easier to rewrite old code than understand and modify it.

It takes experience to judge whether a problem is likely to be hard. Perhaps the quickest way to gain this experience is through careful study of the catalog. Slightly changing the wording of a problem can make the difference between it being polynomial or NP-complete. Finding the shortest path in a graph is easy, while finding the longest path in a graph is hard. Constructing a tour that visits all the edges once in a graph is easy (Eulerian cycle), while constructing a tour that visits all the vertices once is hard (Hamiltonian cycle).

The first thing to do when you suspect a problem might be NP-complete is look in Garey and Johnson's book *Computers and Intractability* [GJ79], which contains a list of several hundred problems known to be NP-complete. Likely you will find the problem you are interested in.

Otherwise I offer the following advice to those seeking to prove the hardness of a given problem:

- *Make your source problem as simple (i.e. , restricted) as possible.*

  Never try to use the general traveling salesman problem (TSP) as a source problem. Better, use Hamiltonian cycle (i.e. , TSP) where all the weights are 1 or ∞. Even better, use Hamiltonian path instead of cycle, so you don't have to worry about closing up the cycle. Best of all, use Hamiltonian path on directed planar graphs where each vertex has total degree 3. All of these problems are equally hard, but the more you can restrict the problem that you are reducing, the less work your reduction has to do.

  As another example, never try to use full satisfiability to prove hardness. Start with 3-satisfiability. In fact, you don't even have to use full 3-satisfiability. Instead, you can use *planar 3-satisfiability*, where there exists a way to draw the clauses as a graph in the plane such that you can connect all instances of the same literal together without edges crossing. This property tends to be useful in proving the hardness of geometric problems. All these problems are equally hard, and hence NP-completeness reductions using any of them are equally convincing.

- *Make your target problem as hard as possible.*

  Don't be afraid to add extra constraints or freedoms to make your target problem more general. Perhaps your undirected graph problem can be generalized into a directed graph problem and can hence be easier to prove hard. Once you have a proof of hardness for the general problem, you can then go back and try to simplify the target.

- *Select the right source problem for the right reason.*

  Selecting the right source problem makes a big difference in how difficult it is to prove a problem hard. This is the first and easiest place to go wrong, although theoretically any NP-complete problem works as well as any other. When trying to prove that a problem is hard, some people fish around through

lists of dozens of problems, looking for the best fit. These people are amateurs; odds are they never will recognize the problem they are looking for when they see it.

I use four (and only four) problems as candidates for my hard source problem. Limiting them to four means that I can know a lot about each of these problems, such as which variants of the problems are hard and which are not. My favorite source problems are:

- *3-SAT*: The old reliable. When none of the three problems below seem appropriate, I go back to the original source.
- *Integer partition*: This is the one and only choice for problems whose hardness seems to require using large numbers.
- *Vertex cover*: This is the answer for any graph problem whose hardness depends upon *selection*. Chromatic number, clique, and independent set all involve trying to select the correct subset of vertices or edges.
- *Hamiltonian path*: This is my choice for any graph problem whose hardness depends upon *ordering*. If you are trying to route or schedule something, Hamiltonian path is likely your lever into the problem.

- *Amplify the penalties for making the undesired selection.*

  Many people are too timid in their thinking about hardness proofs. You are trying to translate one problem into another, while keeping the problems as close to their original identities as as possible. The easiest way to do this is to be bold with your penalties; to punish anyone for trying to deviate from your intended solution. Your thinking should be, "if you select this element, then you must pick up this huge set that prevents you from finding an optimal solution." The sharper the consequences for doing what is undesired, the easier it is to prove the equivalence of the problems.

- *Think strategically at a high level, then build gadgets to enforce tactics.*

  You should be asking yourself the following types of questions: "How can I force that A or B is chosen but not both?" "How can I force that A is taken before B?" "How can I clean up the things I did not select?" Once you have an idea of what you want your gadgets to do, you can worry about how to actually craft them.

- *When you get stuck, alternate between looking for an algorithm or a reduction.*

  Sometimes the reason you cannot prove hardness is that there exists an efficient algorithm to solve your problem! Techniques such as dynamic programming or reducing problems to powerful but polynomial-time graph problems, such as matching or network flow, can yield surprising algorithms. Whenever you can't prove hardness, it pays to alter your opinion occasionally to keep yourself honest.

9.7 War Story: Hard Against the Clock

My class's attention span was running down like sand through an hourglass. Eyes were starting to glaze, even in the front row. Breathing had become soft and regular in the middle of the room. Heads were tilted back and eyes shut in the back.

There were twenty minutes left to go in my lecture on NP-completeness, and I couldn't really blame them. They had already seen several reductions like the ones presented here. But NP-completeness reductions are easier to create than to understand or explain. They had to watch one being created to appreciate how things worked.

I reached for my trusty copy of Garey and Johnson's book [GJ79], which contains a list of over four hundred different known NP-complete problems in an appendix in the back.

"Enough of this!" I announced loudly enough to startle those in the back row. "NP-completeness proofs are sufficiently routine that we can construct them on demand. I need a volunteer with a finger. Can anyone help me?"

A few students in the front held up their hands. A few students in the back held up their fingers. I opted for one from the front row.

"Select a problem at random from the back of this book. I can prove the hardness of any of these problems in the now seventeen minutes remaining in this class. Stick your finger in and read me a problem."

I had definitely gotten their attention. But I could have done that by offering to juggle chain-saws. Now I had to deliver results without cutting myself into ribbons.

The student picked out a problem. "OK, prove that *Inequivalence of Programs with Assignments* is hard," she said.

"Huh? I've never heard of that problem before. What is it? Read me the entire description of the problem so I can write it on the board." The problem was as follows:

Problem: Inequivalence of Programs with Assignments
Input: A finite set X of variables, two programs P_1 and P_2, each a sequence of assignments of the form

$$x_0 \leftarrow \text{ if } (x_1 = x_2) \text{ then } x_3 \text{ else } x_4$$

where the x_i are in X; and a value set V.
Output: Is there an initial assignment of a value from V to each variable in X such that the two programs yield different final values for some variable in X?

I looked at my watch. Fifteen minutes to go. But now everything was on the table. I was faced with a language problem. The input was two programs with variables, and I had to test to see whether they always do the same thing.

"First things first. We need to select a source problem for our reduction. Do we start with integer partition? 3-satisfiability? Vertex cover or Hamiltonian path?"

Since I had an audience, I tried thinking out loud. "Our target is not a graph problem or a numerical problem, so let's start thinking about the old reliable: 3-

satisfiability. There seem to be some similarities. 3-SAT has variables. This thing has variables. To be more like 3-SAT, we could try limiting the variables in this problem so they only take on two values—i.e. , $V = \{\text{true}, \text{false}\}$. Yes. That seems convenient."

My watch said fourteen minutes left. "So, class, which way does the reduction go? 3-SAT to language or language to 3-SAT?"

The front row correctly murmured, "3-SAT to language."

"Right. So we have to translate our set of clauses into two programs. How can we do that? We can try to split the clauses into two sets and write separate programs for each of them. But how do we split them? I don't see any natural way do it, because eliminating any single clause from the problem might suddenly make an unsatisfiable formula satisfiable, thus completely changing the answer. Instead, let's try something else. We can translate all the clauses into one program, and then make the second program be trivial. For example, the second program might ignore the input and always output either only true or only false. This sounds better. *Much* better."

I was still talking out loud to myself, which wasn't that unusual. But I had people listening to me, which was.

"Now, how can we turn a set of clauses into a program? We want to know whether the set of clauses can be satisfied, or if there is an assignment of the variables such that it is true. Suppose we constructed a program to evaluate whether $c_1 = (x_1, \overline{x}_2, x_3)$ is satisfied."

It took me a few minutes worth of scratching before I found the right program to simulate a clause. I assumed that I had access to constants for true and false:

$c_1 =$ if $(x_1 = \text{true})$ then true else false
$c_1 =$ if $(x_2 = \text{false})$ then true else c_1
$c_1 =$ if $(x_3 = \text{true})$ then true else c_1

"Great. Now I have a way to evaluate the truth of each clause. I can do the same thing to evaluate whether all the clauses are satisfied."

$sat =$ if $(c_1 = \text{true})$ then true else false
$sat =$ if $(c_2 = \text{true})$ then sat else false
$\vdots$
$sat =$ if $(c_n = \text{true})$ then sat else false

Now the back of the classroom was getting excited. They were starting to see a ray of hope that they would get to leave on time. There were two minutes left in class.

"Great. So now we have a program that can evaluate to be true if and only if there is a way to assign the variables to satisfy the set of clauses. We need a second program to finish the job. What about $sat = \text{false}$? Yes, that is all we need. Our language problem asks whether the two programs always output the same

thing, regardless of the possible variable assignments. If the clauses are satisfiable, that means that there must be an assignment of the variables such that the long program would output true. Testing whether the programs are equivalent is exactly the same as asking if the clauses are satisfiable."

I lifted my arms in triumph. "And so, the problem is neat, sweet, and NP-complete." I got the last word out just before the bell rang.

9.8 War Story: And Then I Failed

This exercise of picking a random NP-complete problem from the 400+ problems in Garey and Johnson's book and proving hardness on demand was so much fun that I have repeated it each time I have taught the algorithms course. Sure enough, I got it eight times in a row. But just as Joe DiMaggio's 56-game hitting streak came to an end, and Google will eventually have a losing quarter financially, the time came for me to get my comeuppance.

The class had voted to see a reduction from the graph theory section of the catalog, and a randomly selected student picked number 30. Problem GT30 turned out to be:

Problem: Uniconnected Subgraph
Input: Directed graph $G = (V, A)$, positive integer $k \leq |A|$.
Output: Is there a subset of arcs $A' \in A$ with $|A'| \geq k$ such that $G' = (V, A')$ has at most one directed path between any pair of vertices?

"It is a selection problem," I realized as soon as the problem was revealed. After all, we had to select the largest possible subset of arcs so that there were no pair of vertices with multiple paths between them. This meant that vertex cover was the problem of choice.

I worked through how the two problems stacked up. Both sought subsets, although vertex cover wanted subsets of vertices and uniconnected subgraph wanted subsets of edges. Vertex cover wanted the smallest possible subset, while unidirected subgraph wanted the largest possible subset. My source problem had undirected edges while my target had directed arcs, so somehow I would have to add edge direction into the reduction.

I had to do something to direct the edges of the vertex cover graph. I could try to replace each undirected edge (x, y) with a single arc, say from y to x. But quite different directed graphs would result depending upon which direction I selected. Finding the "right" orientation of edges might be a hard problem, certainly too hard to use in the translation phase of the reduction.

I realized I could direct the edges so the resulting graph was a DAG. But then, so what? DAGs certainly can have many different directed paths between pairs of vertices.

Alternately, I could try to replace each undirected edge (x, y) with *two* arcs, from x to y and y to x. Now there was no need to chose the right arcs for my

reduction, but the graph certainly got complicated. I couldn't see how to force things to prevent vertex pairs from having unwanted multiple paths between them.

Meanwhile, the clock was running and I knew it. A sense of panic set in during the last ten minutes of the class, and I realized I wasn't going to get it this time.

There is no feeling worse for a professor than botching up a lecture. You stand up there flailing away, knowing (1) that the students don't understand what you are saying, but (2) they do understand that you also don't understand what you are saying. The bell rang and the students left the room with faces either sympathetic or smirking.

I promised them a solution for the next class, but somehow I kept getting stuck in the same place each time I thought about it. I even tried to cheat and look up the proof in a journal. But the reference that Garey and Johnson cited was a 30-year old unpublished technical report. It wasn't on the web or in our library.

I dreaded the idea of returning to give my next class, the last lecture of the semester. But the night before class the answer came to me in a dream. *"Split the edges,"* the voice said. I awoke with a start and looked at the clock. It was 3:00 AM.

I sat up in bed and scratched out the proof. Suppose I replace each undirected edge (x, y) with a gadget consisting of a new central vertex v_{xy} with arcs going from it to x and y, respectively. This is nice. Now, which vertices are capable of having multiple paths between them? The new vertices had only outgoing edges, so they can only serve as the source of multiple paths. The old vertices had only incoming edges. There was at most one way to get from one of the new source vertices to any of the original vertices of the vertex cover graph, so these could not result in multiple paths.

But now add a sink node s with edges from all original vertices. There were exactly two paths from each new source vertex to this sink—one through each of the two original vertices it was adjacent to. One of these had to be broken to create a uniconnected subgraph. How could we break it? We could pick one of these two vertices to disconnect from the sink by deleting either arc (x, s) or (y, s) for new vertex v_{xy}. We maximize the size of our subgraph by finding the smallest number of arcs to delete. We must delete the outgoing arc from at least one of the two vertices defining each original edge. *This is exactly the same as finding the vertex cover in this graph!* The reduction is illustrated in Figure 9.8.

Presenting this proof in class provided some personal vindication, but more to the point validates the principles I teach for proving hardness. Observe that the reduction really wasn't all that difficult after all: just split the edges and add a sink node. NP-completeness reductions are often surprisingly simple once you look at them the right way.

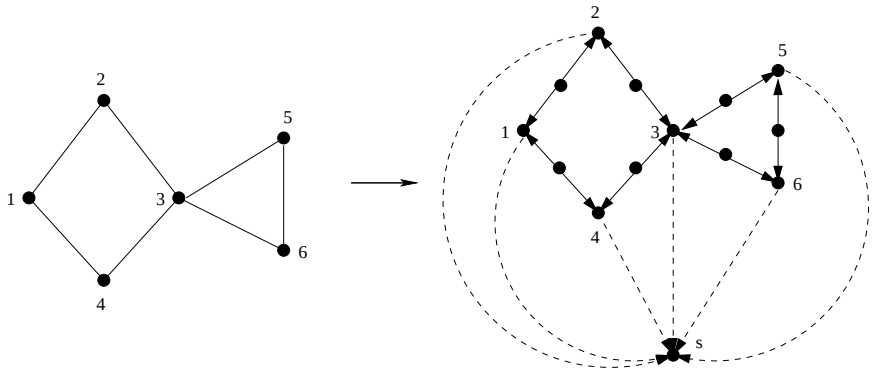


Figure 9.8: Reducing vertex cover to unidirected subgraph, by dividing edges and adding a sink node

9.9 P vs. NP

The theory of NP-completeness rests on a foundation of rigorous but subtle definitions from automata and formal language theory. This terminology is typically confusing to or misused by beginners who lack a mastery of these foundations. It is not really essential to the practical aspects of designing and applying reductions. That said, the question "Is P=NP?" is the most profound open problem in computer science, so any educated algorist should have some idea what the stakes are.

9.9.1 Verification vs. Discovery

The primary question in P vs NP is whether *verification* is really an easier task than initial *discovery*. Suppose that while taking an exam you "happen" to notice the answer of the student next to you. Are you now better off? You wouldn't dare to turn it in without checking, since an able student such as yourself could answer the question correctly if you took enough time to solve it. The issue is whether you can really verify the answer faster than you could find it from scratch.

For the NP-complete decision problems we have studied here, the answer *seems* obvious:

- Can you verify that a graph has a TSP tour of at most k weight given the order of vertices on the tour? Sure. Just add up the weights of the edges on the tour and show it is at most k. That is easier than finding the tour, *isn't it*?
- Can you verify that a given truth assignment represents a solution to a given satisfiability problem? Sure. Just check each clause and make sure it contains

at least one true literal from the given truth assignment. That is easier than finding the satisfying assignment, *isn't it*?

- Can you verify that a graph G has a vertex cover of at most k vertices if given the subset S of at most k vertices forming such a cover? Sure. Just traverse each edge (u, v) of G, and check that either u or v is in S. That is easier than finding the vertex cover, *isn't it*?

At first glance, this seems obvious. The given solutions can be verified in linear time for all three of these problems, while no algorithm faster than brute force search is known to find the solutions for any of them. The catch is that we have no rigorous lower bound *proof* that prevents the existence of fast algorithms to solve these problems. Perhaps there are in fact polynomial algorithms (say $O(n^7)$) that we have just been too blind to see yet.

9.9.2 The Classes P and NP

Every well-defined algorithmic problem must have an asymptotically fastest-possible algorithm solving it, as measured in the Big-Oh, worst-case sense of fastest.

We can think of the class P as an exclusive club for algorithmic problems that a problem can only join after demonstrating that there exists a polynomial-time algorithm to solve it. Shortest path, minimum spanning tree, and the original movie scheduling problem are all members in good standing of this class P. The P stands for *polynomial-time*.

A less-exclusive club welcomes all the algorithmic problems whose solutions can be *verified* in polynomial-time. As shown above, this club contains traveling salesman, satisfiability, and vertex cover, none of which currently have the credentials to join P. However, all the members of P get a free pass into this less exclusive club. If you can solve the problem from scratch in polynomial time, you certainly can verify a solution that fast: just solve it from scratch and see if the solution you get is as good as the one you were given.

We call this less-exclusive club NP. You can think of this as standing for *not-necessarily polynomial-time*.[1]

The $1,000,000 question is whether there are in fact problems in NP that cannot be members of P. If no such problem exists, the classes must be the same and $P = NP$. If even one such a problem exists, the two classes are different and $P \neq NP$. The opinion of most algorists and complexity theorists is that the classes differ, meaning $P \neq NP$, but a much stronger proof than "I can't find a fast enough algorithm" is needed.

[1] In fact, it stands for *nondeterministic polynomial-time*. This is in the sense of nondeterministic automata, if you happen to know about such things.

9.9.3 Why is Satisfiability the Mother of All Hard Problems?

An enormous tree of NP-completeness reductions has been established that entirely rests on the hardness of satisfiability. The portion of this tree demonstrated and/or stated in this chapter (and proven elsewhere) is shown in Figure 9.2.

This may look like a delicate affair. What would it mean if someone *does* find a polynomial-time algorithm for satisfiability? A fast algorithms for any given NP-complete problem (say traveling salesman) implies fast algorithm for all the problems on the path in the reduction tree between TSP and satisfiability (Hamiltonian cycle, vertex cover, and 3-SAT). But a fast algorithm for satisfiability doesn't immediately yield us anything because the reduction path from SAT to SAT is empty.

Fear not. There exists an extraordinary super-reduction (called Cook's theorem) reducing *all* the problems in NP to satisfiability. Thus, if you prove that satisfiability (or equivalently any single NP-complete problem) is in P, then *all* other problems in NP follow and $P = NP$. Since essentially every problem mentioned in this book is in NP, this would be an enormously powerful and surprising result.

Cook's theorem proves that satisfiability is as hard as any problem in NP. Furthermore, it proves that every NP-complete problem is as hard as any other. Any domino falling (i.e. , a polynomial-time algorithm for any NP-complete problem) knocks them all down. Our inability to find a fast algorithm for any of these problems is a strong reason for believing that they are all truly hard, and probably $P \neq NP$.

9.9.4 NP-hard vs. NP-complete?

The final technicality we will discuss is the difference between a problem being NP-hard and NP-complete. I tend to be somewhat loose with my terminology, but there is a subtle (usually irrelevant) distinction between the two concepts.

We say that a problem is *NP-hard* if, like satisfiability, it is at least as hard as any problem in NP. We say that a problem is *NP-complete* if it is NP-hard, and also in NP itself. Because NP is such a large class of problems, most NP-hard problems you encounter will actually be complete, and the issue can always be settled by giving a (usually simple) verification strategy for the problem. All the NP-hard problems we have encountered in this book are also NP-complete.

That said, there are problems that appear to be NP-hard yet not in NP. These problems might be *even harder* than NP-complete! Two-player games such as chess provide examples of problems that are not in NP. Imagine sitting down to play chess with some know-it-all, who is playing white. He pushes his central pawn up two squares to start the game, and announces *checkmate*. The only obvious way to show he is right would be to construct the full tree of all your possible moves with his irrefutable replies and demonstrate that you, in fact, cannot win from the current position. This full tree will have a number of nodes exponential in its height, which is the number of moves before you lose playing your most spirited possible defense.

Clearly this tree cannot be constructed and analyzed in polynomial time, so the problem is not in NP.

9.10 Dealing with NP-complete Problems

For the practical person, demonstrating that a problem is NP-complete is never the end of the line. Presumably, there was a reason why you wanted to solve it in the first place. That application will not go away when told that there is no polynomial-time algorithm. You still seek a program that solves the problem of interest. All you know is that you won't find one that quickly solves the problem to optimality in the worst case. You still have three options:

- *Algorithms fast in the average case* – Examples of such algorithms include backtracking algorithms with substantial pruning.

- *Heuristics* – Heuristic methods like simulated annealing or greedy approaches can be used to quickly find a solution with no guarantee that it will be the best one.

- *Approximation algorithms* – The theory of NP-completeness only stipulates that it is hard to get close to the answer. With clever, problem-specific heuristics, we can probably get *close* to the optimal answer on all possible instances.

Approximation algorithms return solutions with a guarantee attached, namely that the optimal solution can never be much better than this given solution. Thus you can never go too far wrong when using an approximation algorithm. No matter what your input instance is and how lucky you are, you are doomed to do all right. Furthermore, approximation algorithms realizing probably good bounds are often conceptually simple, very fast, and easy to program.

One thing that is usually not clear, however, is how well the solution from an approximation algorithm compares to what you might get from a heuristic that gives you no guarantees. The answer could be worse or it could be better. Leaving your money in a bank savings account guarantees you 3% interest without risk. Still, you likely will do much better investing your money in stocks than leaving it in the bank, even though performance is not guaranteed.

One way to get the best of approximation algorithms and heuristics is to run both of them on the given problem instance and pick the solution giving the better result. This way, you get a solution that comes with a guarantee and a second chance to do even better. When it comes to heuristics for hard problems, sometimes you can have it both ways.

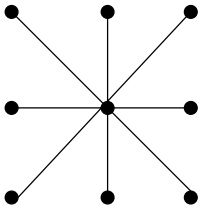


Figure 9.9: Neglecting to pick the center vertex leads to a terrible vertex cover

9.10.1 Approximating Vertex Cover

As we have seen before, finding the minimum vertex cover of a graph is NP-complete. However, a very simple procedure can efficiently find a cover that is at most twice as large as the optimal cover:

VertexCover($G = (V, E)$)
    While ($E \neq \emptyset$) do:
        Select an arbitrary edge $(u, v) \leq E$
        Add both u and v to the vertex cover
        Delete all edges from E that are incident to either u or v.

It should be apparent that this procedure always produces a vertex cover, since each edge is only deleted after an incident vertex has been added to the cover. More interesting is the claim that any vertex cover must use at least half as many vertices as this one. Why? Consider only the $\leq n/2$ edges selected by the algorithm that constitute a matching in the graph. No two of these edges can share a vertex. Therefore, any cover of just these edges must include at least one vertex per edge, which makes it at least half the size of this greedy cover.

There are several interesting things to notice about this algorithm:

- *Although the procedure is simple, it is not stupid* – Many seemingly smarter heuristics can give a far worse performance in the worst case. For example, why not modify the above procedure to select only one of the two vertices for the cover instead of both. After all, the selected edge will be equally well covered by only one vertex. However, consider the star-shaped graph of Figure 9.9. This heuristic will produce a two-vertex cover, while the single-vertex heuristic can return a cover as large as $n - 1$ vertices, should we get unlucky and repeatedly select the leaf instead of the center as the cover vertex we retain.

- *Greedy isn't always the answer* – Perhaps the most natural heuristic for vertex cover would repeatedly select and delete the vertex of highest remaining degree for the vertex cover. After all, this vertex will cover the largest number

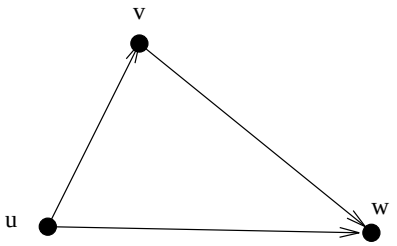


Figure 9.10: The triangle inequality ($d(u,w) \leq d(u,v) + d(v,w)$) typically holds in geometric and weighted graph problems

of possible edges. However, in the case of ties or near ties, this heuristic can go seriously astray. In the worst case, it can yield a cover that is $\Theta(\lg n)$ times optimal.

- *Making a heuristic more complicated does not necessarily make it better* – It is easy to complicate heuristics by adding more special cases or details. For example, the procedure above does not specify which edge should be selected next. It might seem reasonable to next select the edge whose endpoints have the highest degree. However, this does not improve the worst-case bound and just makes it more difficult to analyze.

- *A postprocessing cleanup step can't hurt* – The flip side of designing simple heuristics is that they can often be modified to yield better-in-practice solutions without weakening the approximation bound. For example, a postprocessing step that deletes any unnecessary vertex from the cover can only improve things in practice, even though it won't help the worst-case bound.

The important property of approximation algorithms is relating the size of the solution produced directly to a lower bound on the optimal solution. Instead of thinking about how well we might do, we must think about the worst case—i.e. , how badly we might perform.

9.10.2 The Euclidean Traveling Salesman

In most natural applications of the traveling salesman problem, direct routes are inherently shorter than indirect routes. For example, if a graph's edge weights were the straight-line distances between pairs of cities, the shortest path from x to y will always be "as the crow flies."

The edge weights induced by Euclidean geometry satisfy the triangle inequality, namely that $d(u,w) \leq d(u,v) + d(v,w)$ for all triples of vertices u, v, and w. The general reasonableness of this condition is demonstrated in Figure 9.10. The cost of airfare is an example of a distance function that *violates* the triangle inequality,

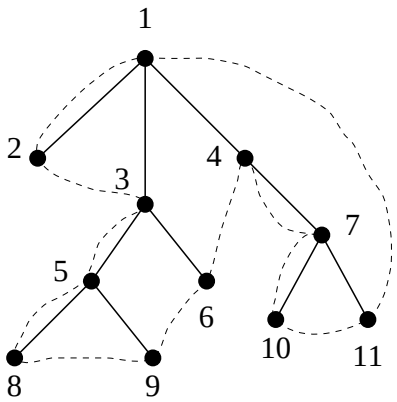


Figure 9.11: A depth-first traversal of a spanning tree, with the shortcut tour

since it is sometimes cheaper to fly through an intermediate city than to fly to the destination directly. TSP remains hard when the distances are Euclidean distances in the plane.

We can approximate the optimal traveling salesman tour using minimum spanning trees or graphs that obey the triangle inequality. First, observe that the weight of a minimum spanning tree is a lower bound on the cost of the optimal tour. Why? Deleting any edge from a tour leaves a path, the total weight of which must be no greater than that of the original tour. This path has no cycles, and hence is a tree, which means its weight is at least that of the minimum spanning tree. Thus the weight of the minimum spanning tree gives a lower bound on the optimal tour.

Consider now what happens in performing a depth-first traversal of a spanning tree. We will visit each edge twice, once going down the tree when discovering the edge and once going up after exploring the entire subtree. For example, in the depth-first search of Figure 9.11, we visit the vertices in order $1-2-1-3-5-8-5-9-5-3-6-3-1-4-7-10-7-11-7-4-1$, thus using every tree edge exactly twice. This tour repeats each edge of the minimum spanning tree twice, and hence costs at most twice the optimal tour.

However, vertices will be repeated on this depth-first search tour. To remove the extra vertices, we can take a shortest path to the next unvisited vertex at each step. The shortcut tour for the tree above is $1-2-3-5-8-9-6-4-7-10-11-1$. Because we have replaced a chain of edges by a single direct edge, the triangle inequality ensures that the tour can only get shorter. Thus, this shortcut tour is also within weight and twice that of optimal. Better, more complicated approximation algorithms for Euclidean TSP exist, as described in Section 16.4 (page 533). No approximation algorithms are known for TSPs that do not satisfy the triangle inequality.

9.10.3 Maximum Acyclic Subgraph

Directed acyclic graphs (DAGs) are easier to work with than general digraphs. Sometimes it is useful to simplify a given graph by deleting a small set of edges or vertices that suffice to break all cycles. Such *feedback set* problems are discussed in Section 16.11 (page 559).

Here we consider an interesting problem in this class where seek to retain as many edges as possible while breaking all directed cycles:

Problem: Maximum Directed Acyclic Subgraph
Input: A directed graph $G = (V, E)$.
Output: Find the largest possible subset $E' \in E$ such that $G' = (V, E')$ is acyclic.

In fact, there is a very simple algorithm that guarantees you a solution with at least half as many edges as optimum. I encourage you to try to find it now before peeking.

Construct *any* permutation of the vertices, and interpret it as a left-right ordering akin to topological sorting. Now some of the edges will point from left to right, while the remainder point from right to left.

One of these two edge subsets must be at least as large as the other. This means it contains at least half the edges. Furthermore each of these two edge subsets must be acyclic for the same reason only DAGs can be topologically sorted—you cannot form a cycle by repeatedly moving in one direction. Thus, the larger edge subset must be acyclic and contain at least half the edges of the optimal solution!

This approximation algorithm *is* simple to the point of almost being stupid. But note that heuristics can make it perform better in practice without losing this guarantee. Perhaps we can try many random permutations, and pick the best. Or we can try to exchange pairs of vertices in the permutations retaining those swaps, which throw more edges onto the bigger side.

9.10.4 Set Cover

The previous sections may encourage a false belief that every problem can be approximated to within a factor of two. Indeed, several catalog problems such as maximum clique cannot be approximated to *any* interesting factor.

Set cover occupies a middle ground between these extremes, having a factor-$\Theta(\lg n)$ approximation algorithm. Set cover is a more general version of the vertex cover problem. As defined in Section 18.1 (page 621),

Problem: Set Cover
Input: A collection of subsets $S = \{S_1, \ldots, S_m\}$ of the universal set $U = \{1, \ldots, n\}$.
Output: What is the smallest subset T of S whose union equals the universal set—i.e. , $\cup_{i=1}^{|T|} T_i = U$?

milestone class	6	5		4					3			2	1	0
uncovered elements	64	51	40	30	25	22	19	16	13	10	7	4	2	1
selected subset size	13	11	10	5	3	3	3	3	3	3	3	2	1	1

Figure 9.12: The coverage process for greedy on a particular instance of set cover

The natural heuristic is greedy. Repeatedly select the subset that covers the largest collection of thus-far uncovered elements until everything is covered. In pseudocode,

```
SetCover(S)
    While (U ≠ ∅) do:
        Identify the subset S_i with the largest intersection with U
        Select S_i for the set cover
        U = U − S_i
```

One consequence of this selection process is that the number of freshly-covered elements defines a nonincreasing sequence as the algorithm proceeds. Why? If not, greedy would have picked the more powerful subset earlier if it, in fact, existed.

Thus we can view this heuristic as reducing the number of uncovered elements from n down to zero by progressively smaller amounts. A trace of such an execution is shown in Figure 9.12.

An important milestone in such a trace occurs each time the number of remaining uncovered elements reduces past a power of two. Clearly there can be at most $\lceil \lg n \rceil$ such events.

Let w_i denote the number of subsets that were selected by the heuristic to cover elements between milestones $2^{i+1} - 1$ and 2^i. Define the width w to be the maximum w_i, where $0 \leq i \leq \lg_2 n$. In the example of Figure 9.12, the maximum width is given by the five subsets needed to go from $2^5 - 1$ down to 2^4.

Since there are at most $\lg n$ such milestones, the solution produced by the greedy heuristic must contain at most $w \cdot \lg n$ subsets. But I claim that the optimal solution must contain *at least* w subsets, so the heuristic solution is no worse than $\lg n$ times optimal.

Why? Consider the average number of new elements covered as we move between milestones $2^{i+1} - 1$ and 2^i. These 2^i elements require w_i subsets, so the average coverage is $\mu_i = 2^i / w_i$. More to the point, the last/smallest of these subsets covers at most μ_i subsets. Thus, *no subset exists in S that can cover more than μ_i of the remaining 2^i elements.* So, to finish the job, we need at least $2^i / \mu_i = w_i$ subsets.

The somewhat surprising thing is that there do exist set cover instances where this heuristic takes $\Omega(\lg n)$ times optimal. The logarithmic factor is a property of the problem/heuristic, not an artifact of weak analysis.

Take-Home Lesson: Approximation algorithms guarantee answers that are always close to the optimal solution. They can provide a practical approach to dealing with NP-complete problems.

Chapter Notes

The notion of NP-completeness was first developed by Cook [Coo71]. Satisfiability really is a $1,000,000 problem, and the Clay Mathematical Institute has offered such a prize to any person who resolves the P=NP question. See *http://www.claymath.org/* for more on the problem and the prize.

Karp [Kar72] showed the importance of Cook's result by providing reductions from satisfiability to more than 20 important algorithmic problems. I recommend Karp's paper for its sheer beauty and economy—he reduces each reduction to three line descriptions showing the problem equivalence. Together, these provided the tools to resolve the complexity of literally hundreds of important problems where no efficient algorithms were known.

The best introduction to the theory of NP-completeness remains Garey and Johnson's book *Computers and Intractability*. It introduces the general theory, including an accessible proof of Cook's theorem [Coo71] that satisfiability is as hard as anything in NP. They also provide an essential reference catalog of more than 300 NP-complete problems, which is a great resource for learning what is known about the most interesting hard problems. The reductions claimed, but missing from this chapter can be found in Garey and Johnson, or textbooks such as [CLRS01].

A few catalog problems exist in a limbo state where it is not known whether the problem has a fast algorithm or is NP-complete. The most prominent of these are graph isomorphism (see Section 16.9 (page 550)) and integer factorization (see Section 13.8 (page 420)). That this limbo list is so short is quite a tribute to the state of the art in algorithm design and the power of NP-completeness. For almost every important problem we either have a fast algorithm or a good solid reason for why one doesn't exist.

The war story problem on unidirected subgraph was originally proven hard in [Mah76].

9.11 Exercises

Transformations and Satisfiability

9-1. *[2]* Give the 3-SAT formula that results from applying the reduction of SAT to 3-SAT for the formula:

$$(x + y + \overline{z} + w + u + \overline{v}) \cdot (\overline{x} + \overline{y} + z + \overline{w} + u + v) \cdot (x + \overline{y} + \overline{z} + w + u + \overline{v}) \cdot (x + \overline{y})$$

9-2. *[3]* Draw the graph that results from the reduction of 3-SAT to vertex cover for the expression

$$(x + \overline{y} + z) \cdot (\overline{x} + y + \overline{z}) \cdot (\overline{x} + y + z) \cdot (x + \overline{y} + \overline{x})$$

9-3. *[4]* Suppose we are given a subroutine which can solve the traveling salesman decision problem of page 318 in, say, linear time. Give an efficient algorithm to find the actual TSP tour by making a polynomial number of calls to this subroutine.

9-4. *[7]* Implement a translator that translates satisfiability instances into equivalent 3-SAT instances.

9-5. *[7]* Design and implement a backtracking algorithm to test whether a set of formulae are satisfiable. What criteria can you use to prune this search?

9-6. *[8]* Implement the vertex cover to satisfiability reduction, and run the resulting clauses through a satisfiability testing code. Does this seem like a practical way to compute things?

Basic Reductions

9-7. *[4]* An instance of the *set cover* problem consists of a set X of n elements, a family F of subsets of X, and an integer k. The question is, does there exist k subsets from F whose union is X?

For example, if $X = \{1, 2, 3, 4\}$ and $F = \{\{1, 2\}, \{2, 3\}, \{4\}, \{2, 4\}\}$, there does not exist a solution for $k = 2$, but there does for $k = 3$ (for example, $\{1, 2\}, \{2, 3\}, \{4\}$).

Prove that set cover is NP-complete with a reduction from vertex cover.

9-8. *[4]* The *baseball card collector problem* is as follows. Given packets $P_1, \ldots, P_m$, each of which contains a subset of this year's baseball cards, is it possible to collect all the year's cards by buying $\leq k$ packets?

For example, if the players are $\{Aaron, Mays, Ruth, Skiena\}$ and the packets are

$$\{\{Aaron, Mays\}, \{Mays, Ruth\}, \{Skiena\}, \{Mays, Skiena\}\},$$

there does not exist a solution for $k = 2$, but there does for $k = 3$, such as

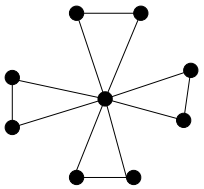
$$\{Aaron, Mays\}, \{Mays, Ruth\}, \{Skiena\}$$

Prove that the baseball card collector problem is NP-hard using a reduction from vertex cover.

9-9. *[4]* The *low-degree spanning tree problem* is as follows. Given a graph G and an integer k, does G contain a spanning tree such that all vertices in the tree have degree *at most* k (obviously, only tree edges count towards the degree)? For example, in the following graph, there is no spanning tree such that all vertices have a degree less than three.

(a) Prove that the low-degree spanning tree problem is NP-hard with a reduction from Hamiltonian *path*.

(b) Now consider the *high-degree spanning tree problem*, which is as follows. Given a graph G and an integer k, does G contain a spanning tree whose highest degree vertex is *at least* k? In the previous example, there exists a spanning tree with a highest degree of 8. Give an efficient algorithm to solve the high-degree spanning tree problem, and an analysis of its time complexity.



9-10. *[4]* Show that the following problem is NP-complete:

Problem: Dense subgraph
Input: A graph G, and integers k and y.
Output: Does G contain a subgraph with exactly k vertices and at least y edges?

9-11. *[4]* Show that the following problem is NP-complete:

Problem: Clique, no-clique
Input: An undirected graph $G = (V, E)$ and an integer k.
Output: Does G contain both a clique of size k and an independent set of size k.

9-12. *[5]* An *Eulerian cycle* is a tour that visits every edge in a graph exactly once. An *Eulerian subgraph* is a subset of the edges and vertices of a graph that has an Eulerian cycle. Prove that the problem of finding the number of edges in the largest Eulerian subgraph of a graph is NP-hard. (Hint: the Hamiltonian circuit problem is NP-hard even if each vertex in the graph is incident upon exactly three edges.)

Creative Reductions

9-13. *[5]* Prove that the following problem is NP-complete:

Problem: Hitting Set
Input: A collection C of subsets of a set S, positive integer k.
Output: Does S contain a subset S' such that $|S'| \leq k$ and each subset in C contains at least one element from S'?

9-14. *[5]* Prove that the following problem is NP-complete:

Problem: Knapsack
Input: A set S of n items, such that the ith item has value v_i and weight w_i. Two positive integers: weight limit W and value requirement V.
Output: Does there exist a subset $S' \in S$ such that $\sum_{i \in S'} w_i \leq W$ and $\sum_{i \in S'} v_i \geq V$? (Hint: start from integer partition.)

9-15. *[5]* Prove that the following problem is NP-complete:

Problem: Hamiltonian Path
Input: A graph G, and vertices s and t.

Output: Does G contain a path which starts from s, ends at t, and visits all vertices without visiting any vertex more than once? (Hint: start from Hamiltonian cycle.)

9-16. *[5]* Prove that the following problem is NP-complete:

Problem: Longest Path
Input: A graph G and positive integer k.
Output: Does G contain a path that visits at least k different vertices without visiting any vertex more than once?

9-17. *[6]* Prove that the following problem is NP-complete:

Problem: Dominating Set
Input: A graph $G = (V, E)$ and positive integer k.
Output: Is there a subset $V' \in V$ such that $|V'| \leq k$ where for each vertex $x \in V$ either $x \in V'$ or there exists an edge (x, y), where $y \in V'$.

9-18. *[7]* Prove that the vertex cover problem (does there exist a subset S of k vertices in a graph G such that every edge in G is incident upon at least one vertex in S?) remains NP-complete even when all the vertices in the graph are restricted to have even degrees.

9-19. *[7]* Prove that the following problem is NP-complete:

Problem: Set Packing
Input: A collection C of subsets of a set S, positive integer k.
Output: Does S contain at least k disjoint subsets (i.e. , such that none of these subsets have any elements in common?)

9-20. *[7]* Prove that the following problem is NP-complete:

Problem: Feedback Vertex Set
Input: A directed graph $G = (V, A)$ and positive integer k.
Output: Is there a subset $V' \in V$ such that $|V'| \leq k$, such that deleting the vertices of V' from G leaves a DAG?

Algorithms for Special Cases

9-21. *[5]* A Hamiltonian path P is a path that visits each vertex exactly once. The problem of testing whether a graph G contains a Hamiltonian path is NP-complete. There does not have to be an edge in G from the ending vertex to the starting vertex of P, unlike in the Hamiltonian cycle problem.

Give an $O(n + m)$-time algorithm to test whether a directed acyclic graph G (a DAG) contains a Hamiltonian path. (Hint: think about topological sorting and DFS.)

9-22. *[8]* The 2-SAT problem is, given a Boolean formula in 2-conjunctive normal form (CNF), to decide whether the formula is satisfiable. 2-SAT is like 3-SAT, except

that each clause can have only two literals. For example, the following formula is in 2-CNF:

$$(x_1 \vee x_2) \wedge (\bar{x}_2 \vee x_3) \wedge (x_1 \vee \bar{x}_3)$$

Give a polynomial-time algorithm to solve 2-SAT.

P=NP?

9-23. *[4]* Show that the following problems are in NP:

- Does graph G have a simple path (i.e. , with no vertex repeated) of length k?
- Is integer n composite (i.e. , not prime)?
- Does graph G have a vertex cover of size k?

9-24. *[7]* It was a long open question whether the decision problem "Is integer n a composite number, in other words, not prime?" can be computed in time polynomial in the size of its input. Why doesn't the following algorithm suffice to prove it is in P, since it runs in $O(n)$ time?

```
PrimalityTesting(n)
    composite := false
    for i := 2 to n − 1 do
        if (n mod i) = 0 then
            composite := true
```

Approximation Algorithms

9-25. *[4]* In the *maximum-satisfiability problem*, we seek a truth assignment that satisfies as many clauses as possible. Give an heuristic that always satisfies at least half as many clauses as the optimal solution.

9-26. *[5]* Consider the following heuristic for vertex cover. Construct a DFS tree of the graph, and delete all the leaves from this tree. What remains must be a vertex cover of the graph. Prove that the size of this cover is at most twice as large as optimal.

9-27. *[5]* The *maximum cut* problem for a graph $G = (V, E)$ seeks to partition the vertices V into disjoint sets A and B so as to maximize the number of edges $(a, b) \in E$ such that $a \in A$ and $b \in B$. Consider the following heuristic for max cut. First assign v_1 to A and v_2 to B. For each remaining vertex, assign it to the side that adds the most edges to the cut. Prove that this cut is at least half as large as the optimal cut.

9-28. *[5]* In the *bin-packing problem*, we are given n items with weights $w_1, w_2, ..., w_n$, respectively. Our goal is to find the smallest number of bins that will hold the n objects, where each bin has capacity of at most one kilogram.

The *first-fit heuristic* considers the objects in the order in which they are given. For each object, place it into first bin that has room for it. If no such bin exists, start a new bin. Prove that this heuristic uses at most twice as many bins as the optimal solution.

9-29. *[5]* For the first-fit heuristic described just above, give an example where the packing it fits uses at least 5/3 times as many bins as optimal.

9-30. *[5]* A *vertex coloring* of graph $G = (V, E)$ is an assignment of colors to vertices of V such that each edge (x, y) implies that vertices x and y are assigned different colors. Give an algorithm for vertex coloring G using at most $\Delta + 1$ colors, where Δ is the maximum vertex degree of G.

Programming Challenges

These programming challenge problems with robot judging are available at *http://www.programming-challenges.com* or *http://online-judge.uva.es*.

Geometry

9-1. "The Monocycle" – Programming Challenges 111202, UVA Judge 10047.

9-2. "Dog and Gopher" – Programming Challenges 10310, UVA Judge 111301.

9-3. "Chocolate Chip Cookies" – Programming Challenges 111304, UVA Judge 10136.

9-4. "Birthday Cake" – Programming Challenges 111305, UVA Judge 10167.

Computational Geometry

9-5. "Closest Pair Problem" – Programming Challenges 111402, UVA Judge 10245.

9-6. "Chainsaw Massacre" – Programming Challenges 111403, UVA Judge 10043.

9-7. "Hotter Colder" – Programming Challenges 111404, UVA Judge 10084.

9-8. "Useless Tile Packers" – Programming Challenges 111405, UVA Judge 10065.

Note: These are not particularly relevant to NP-completeness, but are added for completeness.

10

How to Design Algorithms

Designing the right algorithm for a given application is a major creative act—that of taking a problem and pulling a solution out of the ether. The space of choices you can make in algorithm design is enormous, leaving you plenty of freedom to hang yourself.

This book is designed to make you a better algorithm designer. The techniques presented in Part I of this book provide the basic ideas underlying all combinatorial algorithms. The problem catalog of Part II will help you with modeling your application, and tell you what is known about the relevant problems. However, being a successful algorithm designer requires more than book knowledge. It requires a certain attitude—the right problem-solving approach. It is difficult to teach this mindset in a book, yet getting it is essential to becoming a successful designer.

The key to algorithm design (or any other problem-solving task) is to proceed by asking yourself questions to guide your thought process. *What if we do this? What if we do that?* Should you get stuck on the problem, the best thing to do is move onto the next question. In any group brainstorming session, the most useful person in the room is the one who keeps asking, *"Why can't we do it this way?"* not the person who later tells them why, because she will eventually stumble on an approach that can't be shot down.

Towards this end, we provide a sequence of questions to guide your search for the right algorithm for your problem. To use it effectively, you must not only ask the questions, but answer them. The key is working through the answers carefully by writing them down in a log. The correct answer to *"Can I do it this way?"* is never "no," but "no, because. . . ." By clearly articulating your reasoning as to why something doesn't work, you can check whether you have glossed over a possibility that you didn't want to think hard enough about. It is amazing how often the reason

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you can't find a convincing explanation for something is because your conclusion is wrong.

The distinction between *strategy* and *tactics* is important to keep aware of during any design process. Strategy represents the quest for the big picture—the framework around which we construct our path to the goal. Tactics are used to win the minor battles we must fight along the way. In problem-solving, it is important to check repeatedly whether you are thinking on the right level. If you do not have a global strategy of how you are going to attack your problem, it is pointless to worry about the tactics. An example of a strategic question is "Can I model my application as a graph algorithm problem?" A tactical question might be, "Should I use an adjacency list or adjacency matrix data structure to represent my graph?" Of course, such tactical decisions are critical to the ultimate quality of the solution, but they can be properly evaluated only in light of a successful strategy.

Too many people freeze up in their thinking when faced with a design problem. After reading or hearing the problem, they sit down and realize that they *don't know what to do next*. Avoid this fate. Follow the sequence of questions provided below and in most of the catalog problem sections. We'll *tell* you what to do next!

Obviously, the more experience you have with algorithm design techniques such as dynamic programming, graph algorithms, intractability, and data structures, the more successful you will be at working through the list of questions. Part I of this book has been designed to strengthen this technical background. However, it pays to work through these questions regardless of how strong your technical skills are. The earliest and most important questions on the list focus on obtaining a detailed understanding of your problem and do not require specific expertise.

This list of questions was inspired by a passage in [Wol79]—a wonderful book about the space program entitled *The Right Stuff*. It concerned the radio transmissions from test pilots just before their planes crashed. One might have expected that they would panic, so ground control would hear the pilot yelling *Ahhhhhhhhhhhh* —, terminated only by the sound of smacking into a mountain. Instead, the pilots ran through a list of what their possible actions could be. *I've tried the flaps. I've checked the engine. Still got two wings. I've reset the* —. They had "the Right Stuff." Because of this, they sometimes managed to miss the mountain.

I hope this book and list will provide you with "the Right Stuff" to be an algorithm designer. And I hope it prevents you from smacking into any mountains along the way.

1. Do I really understand the problem?
   (a) What exactly does the input consist of?
   (b) What exactly are the desired results or output?
   (c) Can I construct an input example small enough to solve by hand? What happens when I try to solve it?
   (d) How important is it to my application that I always find the optimal answer? Can I settle for something close to the optimal answer?

(e) How large is a typical instance of my problem? Will I be working on 10 items? 1,000 items? 1,000,000 items?

(f) How important is speed in my application? Must the problem be solved within one second? One minute? One hour? One day?

(g) How much time and effort can I invest in implementation? Will I be limited to simple algorithms that can be coded up in a day, or do I have the freedom to experiment with a couple of approaches and see which is best?

(h) Am I trying to solve a numerical problem? A graph algorithm problem? A geometric problem? A string problem? A set problem? Which formulation seems easiest?

2. Can I find a simple algorithm or heuristic for my problem?

   (a) Will brute force solve my problem *correctly* by searching through all subsets or arrangements and picking the best one?

      i. If so, why am I sure that this algorithm always gives the correct answer?

      ii. How do I measure the quality of a solution once I construct it?

      iii. Does this simple, slow solution run in polynomial or exponential time? Is my problem small enough that this brute-force solution will suffice?

      iv. Am I certain that my problem is sufficiently well defined to actually *have* a correct solution?

   (b) Can I solve my problem by repeatedly trying some simple rule, like picking the biggest item first? The smallest item first? A random item first?

      i. If so, on what types of inputs does this heuristic work well? Do these correspond to the data that might arise in my application?

      ii. On what types of inputs does this heuristic work badly? If no such examples can be found, can I show that it always works well?

      iii. How fast does my heuristic come up with an answer? Does it have a simple implementation?

3. Is my problem in the catalog of algorithmic problems in the back of this book?

   (a) What is known about the problem? Is there an implementation available that I can use?

   (b) Did I look in the right place for my problem? Did I browse through all pictures? Did I look in the index under all possible keywords?

(c) Are there relevant resources available on the World Wide Web? Did I do a Google web and Google Scholar search? Did I go to the page associated with this book, *http://www.cs.sunysb.edu/∼algorith*?

4. Are there special cases of the problem that I know how to solve?

   (a) Can I solve the problem efficiently when I ignore some of the input parameters?

   (b) Does the problem become easier to solve when I set some of the input parameters to trivial values, such as 0 or 1?

   (c) Can I simplify the problem to the point where I *can* solve it efficiently?

   (d) Why can't this special-case algorithm be generalized to a wider class of inputs?

   (e) Is my problem a special case of a more general problem in the catalog?

5. Which of the standard algorithm design paradigms are most relevant to my problem?

   (a) Is there a set of items that can be sorted by size or some key? Does this sorted order make it easier to find the answer?

   (b) Is there a way to split the problem in two smaller problems, perhaps by doing a binary search? How about partitioning the elements into big and small, or left and right? Does this suggest a divide-and-conquer algorithm?

   (c) Do the input objects or desired solution have a natural left-to-right order, such as characters in a string, elements of a permutation, or leaves of a tree? Can I use dynamic programming to exploit this order?

   (d) Are there certain operations being done repeatedly, such as searching, or finding the largest/smallest element? Can I use a data structure to speed up these queries? What about a dictionary/hash table or a heap/priority queue?

   (e) Can I use random sampling to select which object to pick next? What about constructing many random configurations and picking the best one? Can I use some kind of directed randomness like simulated annealing to zoom in on the best solution?

   (f) Can I formulate my problem as a linear program? How about an integer program?

   (g) Does my problem seem something like satisfiability, the traveling salesman problem, or some other NP-complete problem? Might the problem be NP-complete and thus not have an efficient algorithm? Is it in the problem list in the back of Garey and Johnson [GJ79]?

6. Am I still stumped?

   (a) Am I willing to spend money to hire an expert to tell me what to do? If so, check out the professional consulting services mentioned in Section 19.4 (page 664).

   (b) Why don't I go back to the beginning and work through these questions again? Did any of my answers change during my latest trip through the list?

Problem-solving is not a science, but part art and part skill. It is one of the skills most worth developing. My favorite book on problem-solving remains Pólya's *How to Solve It* [P57], which features a catalog of problem-solving techniques that are fascinating to browse through, both before and after you have a problem.

11

A Catalog of Algorithmic Problems

This is a catalog of algorithmic problems that arise commonly in practice. It describes what is known about them and gives suggestions about how best to proceed if the problem arises in your application.

What is the best way to use this catalog? First, think about your problem. If you recall the name, look up the catalog entry in the index or table of contents and start reading. Read through the entire entry, since it contains pointers to other relevant problems. Leaf through the catalog, looking at the pictures and problem names to see if something strikes a chord. Don't be afraid to use the index, for every problem in the book is listed there under several possible keywords and applications. If you *still* don't find something relevant, your problem is either not suitable for attack by combinatorial algorithms or else you don't fully understand it. In either case, go back to step one.

The catalog entries contain a variety of different types of information that have never been collected in one place before. Different fields in each entry present information of practical and historical interest.

To make this catalog more easily accessible, we introduce each problem with a pair of graphics representing the problem instance or input on the left and the result of solving the problem in this instance on the right. We have invested considerable thought in creating stylized examples that illustrate desired behaviors more than just definitions. For example, the minimum spanning tree example illustrates how points can be clustered using minimum spanning trees. We hope that people will be able to flip through the pictures and identify which problems might be relevant to them. We augment these pictures with more formal written input and problem descriptions to eliminate the ambiguity inherent in a purely pictorial representation.

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Once you have identified your problem, the discussion section tells you what you should do about it. We describe applications where the problem is likely to arise and the special issues associated with data from them. We discuss the kind of results you can hope for or expect and, most importantly, what you should do to get them. For each problem, we outline a quick-and-dirty algorithm and provide pointers to more powerful algorithms to try next if the first attempt is not sufficient.

For each problem, we identify available software implementations that are discussed in the implementation field of each entry. Many of these routines are quite good, and they can perhaps be plugged directly into your application. Others maybe inadequate for production use, but they hopefully can provide a good model for your own implementation. In general, the implementations are listed in order of descending usefulness, but we will explicitly recommend the best one available for each problem if a clear winner exists. More detailed information for many of these implementations appears in Chapter 19. Essentially all of the implementations are available via the WWW site associated with this book—reachable at *http://www.cs.sunysb.edu/~algorith*.

Finally, in deliberately smaller print, we discuss the history of each problem and present results of primarily theoretical interest. We have attempted to report the best results known for each problem and point out empirical comparisons of algorithms or survey articles if they exist. This should be of interest to students and researchers, and also to practitioners for whom our recommended solutions prove inadequate and need to know if anything better is possible.

Caveats

This is a catalog of algorithmic problems. It is not a cookbook. It cannot be because there are too many recipes and too many possible variations on what people want to eat. My goal is to point you in the right direction so that you can solve your own problems. I try to identify the issues you will encounter along the way—problems that you will have to work out for yourself. In particular:

- For each problem, I suggest algorithms and directions to attack it. These recommendations are based on my experiences, and are aimed toward what I see as typical applications. I felt it was more important to make concrete recommendations for the masses rather than to try to cover all possible situations. If you don't agree with my advice, don't follow it, but before you ignore me, try to understand the reasoning behind my recommendations and articulate a reason why your application violates my assumptions.

- The implementations I recommend are not necessarily complete solutions to your problem. I point to an implementation whenever I feel it might be more useful to someone than just a textbook description of the algorithm. Some programs are useful only as models for you to write your own codes. Others are embedded in large systems and so might be too painful to extract and run

on their own. Assume that all of them contain bugs. Many are quite serious, so beware.

- Please respect the licensing conditions for any implementations you use commercially. Many of these codes are not open source and have licence restrictions. See Section 19.1 for a further discussion of this issue.
- I would be interested in hearing about your experiences with my recommendations, both positive and negative. I would be especially interested in learning about any other implementations that you know about. Feel free to drop me a line at feedback@algorist.com.

12

Data Structures

Data structures are not so much algorithms as they are the fundamental constructs around which you build your application. Becoming fluent in what the standard data structures can do for you is essential to get full value from them.

This puts data structures slightly out of sync with the rest of the catalog. Perhaps the most useful aspect of it will be the pointers to various implementations and data structure libraries. Many of these data structures are nontrivial to implement well, so the programs we point to will be useful as models even if they do not do exactly what you need. Certain fundamental data structures, like kd-trees and suffix trees, are not as well known as they should be. Hopefully, this catalog will serve to better publicize them.

There are a large number of books on elementary data structures available. My favorites include:

- *Sedgewick* [Sed98] – This comprehensive introduction to algorithms and data structures stands out for the clever and beautiful images of algorithms in action. It comes in C, C++, and Java editions.
- *Weiss* [Wei06] – A nice text, emphasizing data structures more than algorithms. Comes in Java, C, C++, and Ada editions.
- *Goodrich and Tamassia* [GT05] – The Java edition makes particularly good use of the author's Java Data Structures Library (JDSL).

The *Handbook of Data Structures and Applications* [MS05] provides a comprehensive and up-to-date survey of research in data structures. The student who took only an elementary course in data structures is likely to be impressed and surprised by the volume of recent work on the subject.

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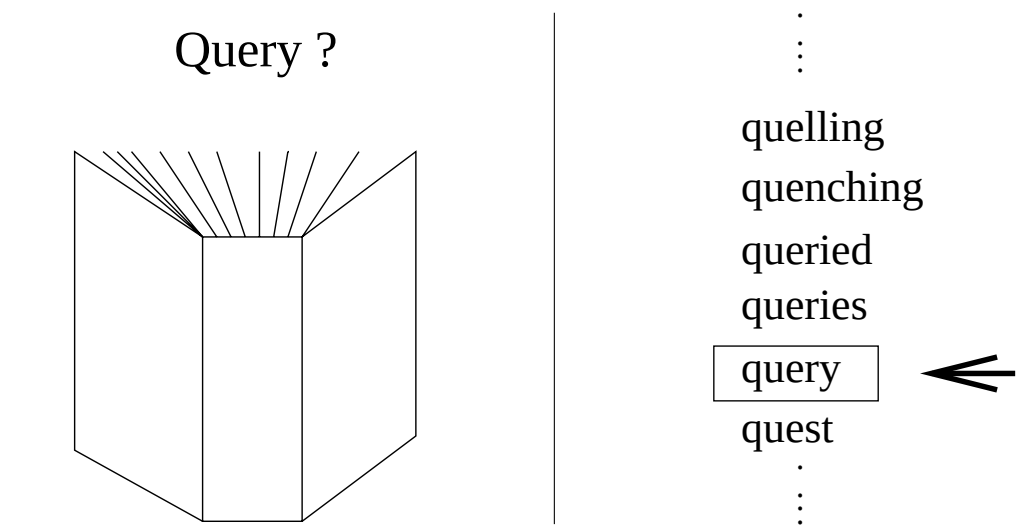


12.1 Dictionaries

Input description: A set of n records, each identified by one or more key fields.

Problem description: Build and maintain a data structure to efficiently locate, insert, and delete the record associated with any query key q.

Discussion: The abstract data type "dictionary" is one of the most important structures in computer science. Dozens of data structures have been proposed for implementing dictionaries, including hash tables, skip lists, and balanced/unbalanced binary search trees. This means that choosing the best one can be tricky. It can significantly impact performance. *However, in practice, it is more important to avoid using a bad data structure than to identify the single best option available.*

An essential piece of advice is to carefully isolate the implementation of the dictionary data structure from its interface. Use explicit calls to methods or subroutines that initialize, search, and modify the data structure, rather than embedding them within the code. This leads to a much cleaner program, but it also makes it easy to experiment with different implementations to see how they perform. Do not obsess about the procedure call overhead inherent in such an abstraction. If your application is so time-critical that such overhead can impact performance, then it is even more essential that you be able to identify the right dictionary implementation.

In choosing the right data structure for your dictionary, ask yourself the following questions:

- *How many items will you have in your data structure?* – Will you know this number in advance? Are you looking at a problem small enough that a simple data structure will suffice, or one so large that we must worry about running out of memory or virtual memory performance?

- *Do you know the relative frequencies of insert, delete, and search operations?* – Static data structures (like sorted arrays) suffice in applications when there are no modifications to the data structure after it is first constructed. *Semi-dynamic* data structures, which support insertion but not deletion, can have significantly simpler implementations than fully dynamic ones.

- *Can we assume that the access pattern for keys will be uniform and random?* – Search queries exhibit a skewed access distribution in many applications, meaning certain elements are much more popular than others. Further, queries often have a sense of temporal locality, meaning elements are likely to be repeatedly accessed in clusters instead of at fairly regular intervals. Certain data structures (such as splay trees) can take advantage of a skewed and clustered universe.

- *Is it critical that individual operations be fast, or only that the total amount of work done over the entire program be minimized?* – When response time is critical, such as in a program controlling a heart-lung machine, you can't wait too long between steps. When you have a program that is doing a lot of queries over the database, such as identifying all criminals who happen to be politicians, it is not as critical that you pick out any particular congressman quickly as it is that you get them all with the minimum total effort.

An object-oriented generation has emerged as no more likely to write a container class than fix the engine in their car. This is good; default containers should do just fine for most applications. Still, it is good sometimes to know what you have under the hood:

- *Unsorted linked lists or arrays* – For small data sets, an unsorted array is probably the easiest data structure to maintain. Linked structures can have terrible cache performance compared with sleek, compact arrays. However, once your dictionary becomes larger than (say) 50 to 100 items, the linear search time will kill you for either lists or arrays. Details of elementary dictionary implementations appear in Section 3.3 (page 72).

  A particularly interesting and useful variant is the *self-organizing list*. Whenever a key is accessed or inserted, we always move it to head of the list. Thus, if the key is accessed again sometime in the near future, it will be near the front and so require only a short search to find it. Most applications exhibit

both uneven access frequencies and locality of reference, so the average time for a successful search in a self-organizing list is typically much better than in a sorted or unsorted list. Of course, self-organizing data structures can be built from arrays as well as linked lists and trees.

- *Sorted linked lists or arrays* – Maintaining a sorted linked list is usually not worth the effort unless you are trying to eliminate duplicates, since we cannot perform binary searches in such a data structure. A sorted array will be appropriate if and only if there are not many insertions or deletions.

- *Hash tables* – For applications involving a moderate-to-large number of keys (say between 100 and 10,000,000), a hash table is probably the right way to go. We use a function that maps keys (be they strings, numbers, or whatever) to integers between 0 and $m-1$. We maintain an array of m buckets, each typically implemented using an unsorted linked list. The hash function immediately identifies which bucket contains a given key. If we use a hash function that spreads the keys out nicely, and a sufficiently large hash table, each bucket should contain very few items, thus making linear searches acceptable. Insertion and deletion from a hash table reduce to insertion and deletion from the bucket/list. Section 3.7 (page 89) provides a more detailed discussion of hashing and its applications.

  A well-tuned hash table will outperform a sorted array in most applications. However, several design decisions go into creating a well-tuned hash table:

  - *How do I deal with collisions?:* Open addressing can lead to more concise tables with better cache performance than bucketing, but performance will be more brittle as the load factor (ratio of occupancy to capacity) of the hash table starts to get high.
  - *How big should the table be?:* With bucketing, m should about the same as the maximum number of items you expect to put in the table. With open addressing, make it (say) 30% larger or more. Selecting m to be a prime number minimizes the dangers of a bad hash function.
  - *What hash function should I use?:* For strings, something like

    $$H(S,j) = \sum_{i=0}^{m-1} \alpha^{m-(i+1)} \times char(s_{i+j}) \bmod m$$

    should work, where α is the size of the alphabet and *char(x)* is the function that maps each character x to its ASCII character code. Use Horner's rule (or precompute values of α^x) to implement this hash function computation efficiently, as discussed in Section 13.9 (page 423). This hash function has the nifty property that

    $$H(S,j+1) = (H(S,j) - \alpha^{m-1} char(s_j))\alpha + s_{j+m}$$

so hash codes of successive m-character windows of a string can be computed in constant time instead of $O(m)$.

Regardless of which hash function you decide to use, print statistics on the distribution of keys per bucket to see how uniform it *really* is. Odds are the first hash function you try will not prove to be the best. Botching up the hash function is an excellent way to slow down any application.

- *Binary search trees* – Binary search trees are elegant data structures that support fast insertions, deletions, and queries. They are reviewed in Section 3.4 (page 77). The big distinction between different types of trees is whether they are explicitly rebalanced after insertion or deletion, and how this rebalancing is done. In *random search trees*, we simply insert a node at the leaf position where we can find it and no rebalancing takes place. Although such trees perform well under random insertions, most applications are not really random. Indeed, unbalanced search trees constructed by inserting keys in sorted order are a disaster, performing like a linked list.

  Balanced search trees use local *rotation* operations to restructure search trees, moving more distant nodes closer to the root while maintaining the in-order search structure of the tree. Among balanced search trees, AVL and 2/3 trees are now passé, and *red-black trees* seem to be more popular. A particularly interesting self-organizing data structure is the *splay tree*, which uses rotations to move any accessed key to the root. Frequently used or recently accessed nodes thus sit near the top of the tree, allowing faster searches.

  Bottom line: Which tree is best for your application? Probably the one of which you have the best implementation. The flavor of balanced tree is probably not as important as the skill of the programmer who coded it.

- *B-trees* – For data sets so large that they will not fit in main memory (say more than 1,000,000 items) your best bet will be some flavor of a B-tree. Once a data structure has to be stored outside of main memory, the search time grows by several orders of magnitude. With modern cache architectures, similar effects can also happen on a smaller scale, since cache is much faster than RAM.

  The idea behind a B-tree is to collapse several levels of a binary search tree into a single large node, so that we can make the equivalent of several search steps before another disk access is needed. With B-tree we can access enormous numbers of keys using only a few disk accesses. To get the full benefit from using a B-tree, it is important to understand how the secondary storage device and virtual memory interact, through constants such as page size and virtual/real address space. *Cache-oblivious algorithms* (described below) can mitigate such concerns.

Even for modest-sized data sets, unexpectedly poor performance of a data structure may result from excessive swapping, so listen to your disk to help decide whether you should be using a B-tree.

- *Skip lists* – These are somewhat of a cult data structure. A hierarchy of sorted linked lists is maintained, where a coin is flipped for each element to decide whether it gets copied into the next highest list. This implies roughly $\lg n$ lists, each roughly half as large as the one above it. Search starts in the smallest list. The search key lies in an interval between two elements, which is then explored in the next larger list. Each searched interval contains an expected constant number of elements per list, for a total expected $O(\lg n)$ query time. The primary benefits of skip lists are ease of analysis and implementation relative to balanced trees.

Implementations: Modern programming languages provide libraries offering complete and efficient container implementations. The C++ *Standard Template Library* (STL) is now provided with most compliers, and available with documentation at *http://www.sgi.com/tech/stl/*. See Josuttis [Jos99], Meyers [Mey01], and Musser [MDS01] for more detailed guides to using STL and the C++ standard library.

LEDA (see Section 19.1.1 (page 658)) provides an extremely complete collection of dictionary data structures in C++, including hashing, perfect hashing, B-trees, red-black trees, random search trees, and skip lists. Experiments reported in [MN99] identified hashing as the best dictionary choice, with skip lists and 2-4 trees (a special case of B-trees) as the most efficient tree-like structures.

Java Collections (JC), a small library of data structures, is included in the `java.util` package of Java standard edition (*http://java.sun.com/javase/*). The *Data Structures Library in Java* (JDSL) is more comprehensive, and available for non-commercial use at *http://www.jdsl.org/*. See [GTV05, GT05] for more detailed guides to JDSL.

Notes: Knuth [Knu97a] provides the most detailed analysis and exposition on fundamental dictionary data structures, but misses certain modern data structures as red-black and splay trees. Spending some time with his books is a worthwhile rite of passage for all computer science students.

The Handbook of Data Structures and Applications [MS05] provides up-to-date surveys on all aspects of dictionary data structures. Other surveys include Mehlhorn and Tsakalidis [MT90b] and Gonnet and Baeza-Yates [GBY91]. Good textbook expositions on dictionary data structures include Sedgewick [Sed98], Weiss [Wei06], and Goodrich/Tamassia [GT05]. We defer to all these sources to avoid giving original references for each of the data structures described above.

The 1996 DIMACS implementation challenge focused on elementary data structures, including dictionaries [GJM02]. Data sets, and codes are accessible from *http://dimacs.rutgers.edu/Challenges*.

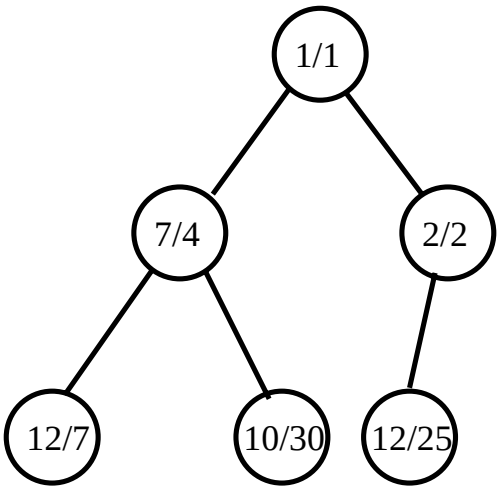
The cost of transferring data back and forth between levels of the memory hierarchy (RAM-to-cache or disk-to-RAM) dominates the cost of actual computation for many

problems. Each data transfer moves one block of size b, so efficient algorithms seek to minimize the number of block transfers. The complexity of fundamental algorithm and data structure problems on such an external memory model has been extensively studied [Vit01]. *Cache-oblivious* data structures offer performance guarantees under such a model without explicit knowledge of the block-size parameter b. Hence, good performance can be obtained on any machine without architecture-specific tuning. See [ABF05] for an excellent survey on cache-oblivious data structures.

Several modern data structures, such as splay trees, have been studied using *amortized analysis*, where we bound the total amount of time used by any sequence of operations. In an amortized analysis, a single operation can be very expensive, but only because we have already benefited from enough cheap operations to pay off the higher cost. A data structure realizing an amortized complexity of $O(f(n))$ is less desirable than one whose worst-case complexity is $O(f(n))$ (since a very bad operation might still occur) but better than one with an average-case complexity $O(f(n))$, since the amortized bound will achieve this average on any input.

Related Problems: Sorting (see page 436), searching (see page 441).

October 30
December 7
July 4
January 1
February 2
December 25



INPUT OUTPUT

12.2 Priority Queues

Input description: A set of records with numerically or otherwise totally-ordered keys.

Problem description: Build and maintain a data structure for providing quick access to the *smallest* or *largest* key in the set.

Discussion: Priority queues are useful data structures in simulations, particularly for maintaining a set of future events ordered by time. They are called "priority" queues because they enable you to retrieve items not by the insertion time (as in a stack or queue), nor by a key match (as in a dictionary), but by which item has the highest priority of retrieval.

If your application will perform no insertions after the initial query, there is no need for an explicit priority queue. Simply sort the records by priority and proceed from top to bottom, maintaining a pointer to the last record retrieved. This situation occurs in Kruskal's minimum spanning tree algorithm, or when simulating a completely scripted set of events.

However, if you are mixing insertions, deletions, and queries, you will need a real priority queue. The following questions will help select the right one:

- *What other operations do you need?* – Will you be searching for arbitrary keys, or just searching for the smallest? Will you be deleting arbitrary elements from the data, or just repeatedly deleting the top or smallest element?

- *Do you know the maximum data structure size in advance?* – The issue here is whether you can preallocate space for the data structure.
- *Might you change the priority of elements already in the queue?* – Changing the priority of elements implies that we must be able to retrieve elements from the queue based on their key, in addition to being able to retrieve the largest element.

Your choices are between the following basic priority queue implementations:

- *Sorted array or list* – A sorted array is very efficient to both identify the smallest element and delete it by decrementing the top index. However, maintaining the total order makes inserting new elements slow. Sorted arrays are only suitable when there will be few insertions into the priority queue. Basic priority queue implementations are reviewed in Section 3.5 (page 83).
- *Binary heaps* – This simple, elegant data structure supports both insertion and extract-min in $O(\lg n)$ time each. Heaps maintain an implicit binary tree structure in an array, such that the key of the root of any subtree is less than that of all its descendents. Thus, the minimum key always sits at the top of the heap. New keys can be inserted by placing them at an open leaf and percolating the element upwards until it sits at its proper place in the partial order. An implementation of binary heap construction and retrieval in C appears in Section 4.3.1 (page 109)

  Binary heaps are the right answer when you know an upper bound on the number of items in your priority queue, since you must specify array size at creation time. Even this constraint can be mitigated by using dynamic arrays (see Section 3.1.1 (page 66)).
- *Bounded height priority queue* – This array-based data structure permits constant-time insertion and find-min operations whenever the range of possible key values is limited. Suppose we know that all key values will be integers between 1 and n. We can set up an array of n linked lists, such that the ith list serves as a bucket containing all items with key i. We will maintain a *top* pointer to the smallest nonempty list. To insert an item with key k into the priority queue, add it to the kth bucket and set $top = \min(top, k)$. To extract the minimum, report the first item from bucket *top*, delete it, and move *top* down if the bucket has become empty.

  Bounded height priority queues are very useful in maintaining the vertices of a graph sorted by degree, which is a fundamental operation in graph algorithms. Still, they are not as widely known as they should be. They are usually the right priority queue for any small, discrete range of keys.
- *Binary search trees* – Binary search trees make effective priority queues, since the smallest element is always the leftmost leaf, while the largest element is

always the rightmost leaf. The min (max) is found by simply tracing down left (right) pointers until the next pointer is nil. Binary tree heaps prove most appropriate when you need other dictionary operations, or if you have an unbounded key range and do not know the maximum priority queue size in advance.

- *Fibonacci and pairing heaps* – These complicated priority queues are designed to speed up *decrease-key* operations, where the priority of an item already in the priority queue is reduced. This arises, for example, in shortest path computations when we discover a shorter route to a vertex v than previously established.

  Properly implemented and used, they lead to better performance on very large computations.

Implementations: Modern programming languages provide libraries offering complete and efficient priority queue implementations. Member functions `push`, `top`, and `pop` of the C++ *Standard Template Library* (STL) `priority_queue` template mirror heap operations `insert`, `findmax`, and `deletemax`. STL is available with documentation at *http://www.sgi.com/tech/stl/*. See Meyers [Mey01] and Musser [MDS01] for more detailed guides to using STL.

LEDA (see Section 19.1.1 (page 658)) provides a complete collection of priority queues in C++, including Fibonacci heaps, pairing heaps, Emde-Boas trees, and bounded height priority queues. Experiments reported in [MN99] identified simple binary heaps as quite competitive in most applications, with pairing heaps beating Fibonacci heaps in head-to-head tests.

The *Java Collections* `PriorityQueue` class is included in the java.util package of Java standard edition (*http://java.sun.com/javase/*). The *Data Structures Library in Java* (JDSL) provides an alternate implementation, and is available for non-commercial use at *http://www.jdsl.org/*. See [GTV05, GT05] for more detailed guides to JDSL.

Sanders [San00] did extensive experiments demonstrating that his sequence heap, based on k-way merging, was roughly twice as fast as a well-implemented binary heap. See *http://www.mpi-inf.mpg.de/∼sanders/programs/spq/* for his implementations in C++.

Notes: *The Handbook of Data Structures and Applications* [MS05] provides several up-to-date surveys on all aspects of priority queues. Empirical comparisons between priority queue data structures include [CGS99, GBY91, Jon86, LL96, San00].

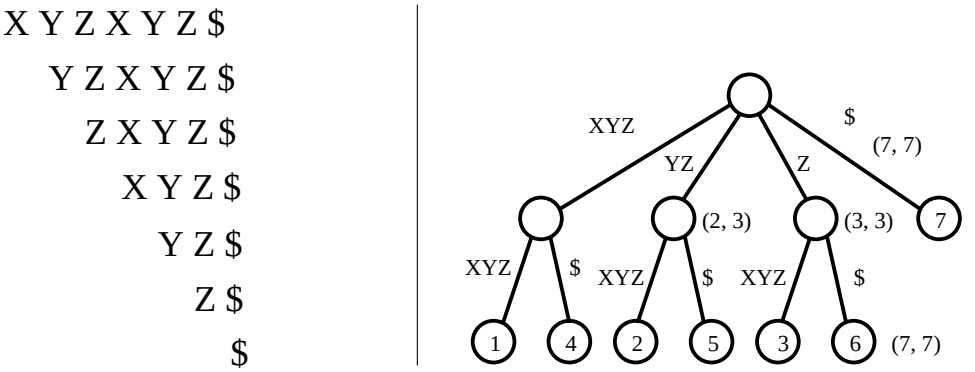
Double-ended priority queues extend the basic heap operations to simultaneously support both find-min and find-max. See [Sah05] for a survey of four different implementations of double-ended priority queues.

Bounded-height priority queues are useful data structures in practice, but do not promise good worst-case performance when arbitrary insertions and deletions are permitted. However, von Emde Boas priority queues [vEBKZ77] support $O(\lg \lg n)$ insertion, deletion, search, max, and min operations where each key is an element from 1 to n.

Fibonacci heaps [FT87] support insert and decrease-key operations in constant amortized time, with $O(\lg n)$ amortized time extract-min and delete operations. The constant-time decrease-key operation leads to faster implementations of classical algorithms for shortest-paths, weighted bipartite-matching, and minimum spanning tree. In practice, Fibonacci heaps are difficult to implement and have large constant factors associated with them. However, pairing heaps appear to realize the same bounds with less overhead. Experiments with pairing heaps are reported in [SV87].

Heaps define a partial order that can be built using a linear number of comparisons. The familiar linear-time merging algorithm for heap construction is due to Floyd [Flo64]. In the worst case, $1.625n$ comparisons suffice [GM86] and $1.5n - O(\lg n)$ comparisons are necessary [CC92].

Related Problems: Dictionaries (see page 367), sorting (see page 436), shortest path (see page 489).



INPUT OUTPUT

12.3 Suffix Trees and Arrays

Input description: A reference string S.

Problem description: Build a data structure to quickly find all places where an arbitrary query string q occurs in S.

Discussion: Suffix trees and arrays are phenomenally useful data structures for solving string problems elegantly and efficiently. Proper use of suffix trees often speeds up string processing algorithms from $O(n^2)$ to linear time—likely the answer. Indeed, suffix trees are the hero of the war story reported in Section 3.9 (page 94).

In its simplest instantiation, a suffix tree is simply a *trie* of the n suffixes of an n-character string S. A trie is a tree structure, where each edge represents one character, and the root represents the null string. Thus, each path from the root represents a string, described by the characters labeling the edges traversed. Any finite set of words defines a trie, and two words with common prefixes branch off from each other at the first distinguishing character. Each leaf denotes the end of a string. Figure 12.1 illustrates a simple trie.

Tries are useful for testing whether a given query string q is in the set. We traverse the trie from the root along branches defined by successive characters of q. If a branch does not exist in the trie, then q cannot be in the set of strings. Otherwise we find q in $|q|$ character comparisons *regardless* of how many strings are in the trie. Tries are very simple to build (repeatedly insert new strings) and very fast to search, although they can be expensive in terms of memory.

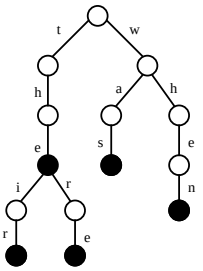


Figure 12.1: A trie on strings *the, their, there, was,* and *when*

A *suffix tree* is simply a trie of all the proper suffixes of S. The suffix tree enables you to test whether q is a substring of S, because any substring of S is the prefix of some suffix (got it?). The search time is again linear in the length of q.

The catch is that constructing a full suffix tree in this manner can require $O(n^2)$ time and, even worse, $O(n^2)$ space, since the average length of the n suffixes is $n/2$. However, linear space suffices to represent a full suffix tree, if we are clever. Observe that most of the nodes in a trie-based suffix tree occur on simple paths between branch nodes in the tree. Each of these simple paths corresponds to a substring of the original string. By storing the original string in an array and collapsing each such path into a single edge, we have all the information of the full suffix tree in only $O(n)$ space. The label for each edge is described by the starting and ending array indices representing the substring. The output figure for this section displays a collapsed suffix tree in all its glory.

Even better, there exist $O(n)$ algorithms to construct this collapsed tree, by making clever use of pointers to minimize construction time. These additional pointers can also be used to speed up many applications of suffix trees.

But what can you do with suffix trees? Consider the following applications. For more details see the books by Gusfield [Gus97] or Crochemore and Rytter [CR03]:

- *Find all occurrences of q as a substring of S* – Just as with a trie, we can walk from the root to the node n_q associated with q. The positions of all occurrences of q in S are represented by the descendents of n_q, which can be identified using a depth-first search from n_q. In collapsed suffix trees, it takes $O(|q| + k)$ time to find the k occurrences of q in S.

- *Longest substring common to a set of strings* – Build a single collapsed suffix tree containing all suffixes of all strings, with each leaf labeled with its original string. In the course of doing a depth-first search on this tree, we can label each node with both the length of its common prefix and the number of distinct strings that are children of it. From this information, the best node can be selected in linear time.

- *Find the longest palindrome in S* – A *palindrome* is a string that reads the same if the order of characters is reversed, such as *madam*. To find the longest palindrome in a string S, build a single suffix tree containing all suffixes of S and the reversal of S, with each leaf identified by its starting position. A palindrome is defined by any node in this tree that has forward and reversed children from the same position.

Since linear time suffix tree construction algorithms are nontrivial, I recommend using an existing implementation. Another good option is to use suffix arrays, discussed below.

Suffix arrays do most of what suffix trees do, while using roughly four times less memory. They are also easier to implement. A suffix array is in principle just an array that contains all the n suffixes of S in sorted order. Thus a binary search of this array for string q suffices to locate the prefix of a suffix that matches q, permitting an efficient substring search in $O(\lg n)$ string comparisons. With the addition of an index specifying the common prefix length of all bounding suffixes, only $\lg n + |q|$ *character* comparisons need be performed on any query, since we can identify the next character that must be tested in the binary search. For example, if the lower range of the search is *cowabunga* and the upper range is *cowslip*, all keys in between must share the same first three letters, so only the fourth character of any intermediate key must be tested against q. In practice, suffix arrays are typically as fast or faster to search than suffix trees.

Suffix arrays use less memory than suffix trees. Each suffix is represented completely by its unique starting position (from 1 to n) and read off as needed using a single reference copy of the input string.

Some care must be taken to construct suffix arrays efficiently, however, since there are $O(n^2)$ characters in the strings being sorted. One solution is to first build a suffix *tree*, then perform an in-order traversal of it to read the strings off in sorted order! However, recent breakthroughs have lead to space/time efficient algorithms for constructing suffix arrays directly.

Implementations: There now exist a wealth of suffix array implementations available. Indeed, all of the recent linear time construction algorithms have been implemented and benchmarked [PST07]. Schürmann and Stoye [SS07] provide an excellent C implementation at *http://bibiserv.techfak.uni-bielefeld.de/bpr/*.

No less than eight different C/C++ implementations of compressed text indexes appear at the *Pizza&Chili corpus* (*http://pizzachili.di.unipi.it/*). These data structures go to great lengths to minimize space usage, typically compressing the input string to near the empirical entropy while still achieving excellent query times!

Suffix tree implementations are also readily available. A `SuffixTree` class is provided in BioJava (*ttp://www.biojava.org/*)—an open source project providing a Java framework for processing biological data. `Libstree` is a C implementation of Ukkonen's algorithm, available at *http://www.icir.org/christian/libstree/*.

Nelson's C++ code [Nel96] is available from *http://marknelson.us/1996/08/01/suffix-trees/*.

Strmat is a collection of C programs implementing exact pattern matching algorithms in association with [Gus97], including an implementation of suffix trees. It is available at *http://www.cs.ucdavis.edu/~gusfield/strmat.html*.

Notes: Tries were first proposed by Fredkin [Fre62], the name coming from the central letters of the word "retrieval." A survey of basic trie data structures with extensive references appears in [GBY91].

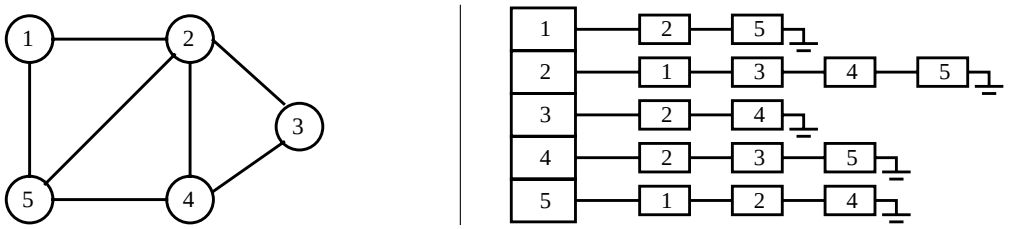
Efficient algorithms for suffix tree construction are due to Weiner [Wei73], McCreight [McC76], and Ukkonen [Ukk92]. Good expositions on these algorithms include Crochmore and Rytter [CR03] and Gusfield [Gus97].

Suffix arrays were invented by Manber and Myers [MM93], although an equivalent idea called *Pat trees* due to Gonnet and Baeza-Yates appears in [GBY91]. Three teams independently emerged with linear-time suffix array algorithms in 2003 [KSPP03, KA03, KSB05], and progress has continued rapidly. See [PST07] for a recent survey covering all these developments.

Recent work has resulted in the development of compressed full text indexes that offer essentially all the power of suffix trees/arrays in a data structure whose size is proportional to the *compressed* text string. Makinen and Navarro [MN07] survey these remarkable data structures.

The power of suffix trees can be further augmented by using a data structure for computing the *least common ancestor (LCA)* of any pair of nodes x, y in a tree in constant time, after linear-time preprocessing of the tree. The original data structure due to Harel and Tarjan [HT84], has been progressively simplified by Schieber and Vishkin [SV88] and later Bender and Farach [BF00]. Expositions include Gusfield [Gus97]. The least common ancestor of two nodes in a suffix tree or trie defines the node representing the longest common prefix of the two associated strings. That we can answer such queries in constant time is amazing, and proves useful as a building block for many other algorithms.

Related Problems: String matching (see page 628), text compression (see page 637), longest common substring (see page 650).



INPUT OUTPUT

12.4 Graph Data Structures

Input description: A graph G.

Problem description: Represent the graph G using a flexible, efficient data structure.

Discussion: The two basic data structures for representing graphs are *adjacency matrices* and *adjacency lists*. Full descriptions of these data structures appear in Section 5.2 (page 151), along with an implementation of adjacency lists in C. In general, for most things, adjacency lists are the way to go.

The issues in deciding which data structure to use include:

- *How big will your graph be?* – How many vertices will it have, both typically and in the worse case? Ditto for the number of edges? Graphs with 1,000 vertices imply adjacency matrices with 1,000,000 entries. This seems too be the boundary of reality. Adjacency matrices make sense only for small or very dense graphs.

- *How dense will your graph be?* – If your graph is very dense, meaning that a large fraction of the vertex pairs define edges, there is probably no compelling reason to use adjacency lists. You will be doomed to using $\Theta(n^2)$ space anyway. Indeed, for complete graphs, matrices will be more concise due to the elimination of pointers.

- *Which algorithms will you be implementing?* – Certain algorithms are more natural on adjacency matrices (such as all-pairs shortest path) and others favor adjacency lists (such as most DFS-based algorithms). Adjacency matrices win for algorithms that repeatedly ask, "Is (i, j) in G?" However, most graph algorithms can be designed to eliminate such queries.

- *Will you be modifying the graph over the course of your application?* – Efficient *static graph* implementations can be used when no edge insertion/deletion operations will done following initial construction. Indeed, more

common than modifying the topology of the graph is modifying the *attributes* of a vertex or edge of the graph, such as size, weight, label, or color. Attributes are best handled as extra fields in the vertex or edge records of adjacency lists.

Building a good general purpose graph type is a substantial project. For this reason, we suggest that you check out existing implementations (particularly LEDA) before hacking up your own. Note that it costs only time linear in the size of the larger data structure to convert between adjacency matrices and adjacency lists. This conversion is unlikely to be the bottleneck in any application, so you may decide to use both data structures if you have the space to store them. This usually isn't necessary, but might prove simplest if you are confused about the alternatives.

Planar graphs are those that can be drawn in the plane so no two edges cross. Graphs arising in many applications are planar by definition, such as maps of countries. Others are planar by happenstance, like trees. Planar graphs are always sparse, since any n-vertex planar graph can have at most $3n - 6$ edges. Thus they should be represented using adjacency lists. If the planar drawing (or *embedding*) of the graph is fundamental to what is being computed, planar graphs are best represented geometrically. See Section 15.12 (page 520) for algorithms for constructing planar embeddings from graphs. Section 17.15 (page 614) discusses algorithms for maintaining the graphs implicit in the arrangements of geometric objects like lines and polygons.

Hypergraphs are generalized graphs where each edge may link subsets of more than two vertices. Suppose we want to represent who is on which Congressional committee. The vertices of our hypergraph would be the individual congressmen, while each hyperedge would represent one committee. Such arbitrary collections of subsets of a set are naturally thought of as hypergraphs.

Two basic data structures for hypergraphs are:

- *Incidence matrices*, which are analogous to adjacency matrices. They require $n \times m$ space, where m is the number of hyperedges. Each row corresponds to a vertex, and each column to an edge, with a nonzero entry in $M[i, j]$ iff vertex i is incident to edge j. On standard graphs there are two nonzero entries in each column. The degree of each vertex governs the number of nonzero entries in each row.

- *Bipartite incidence structures*, which are analogous to adjacency lists, and hence suited for sparse hypergraphs. There is a vertex of the incidence structure associated with each edge and vertex of the hypergraphs, and an edge (i, j) in the incidence structure if vertex i of the hypergraph appears in edge j of the hypergraph. Adjacency lists are typically used to represent this incidence structure. Drawing the associated bipartite graph provides a natural way to visualize the hypergraph.

Special efforts must be taken to represent very large graphs efficiently. However, interesting problems have been solved on graphs with millions of edges and

vertices. The first step is to make your data structure as lean as possible, by packing your adjacency matrix in a bit vector (see Section 12.5 (page 385)) or removing unnecessary pointers from your adjacency list representation. For example, in a static graph (which does not support edge insertions or deletions) each edge list can be replaced by a packed array of vertex identifiers, thus eliminating pointers and potentially saving half the space.

If your graph is extremely large, it may become necessary to switch to a hierarchical representation, where the vertices are clustered into subgraphs that are compressed into single vertices. Two approaches exist to construct such a hierarchical decomposition. The first breaks the graph into components in a natural or application-specific way. For example, a graph of roads and cities suggests a natural decomposition—partition the map into districts, towns, counties, and states. The other approach runs a graph partition algorithm discussed as in Section 16.6 (page 541). If you have one, a natural decomposition will likely do a better job than some naive heuristic for an NP-complete problem. If your graph is really unmanageably large, you cannot afford to do a very good job of algorithmically partitioning it. First verify that standard data structures fail on your problem before attempting such heroic measures.

Implementations: LEDA (see Section 19.1.1 (page 658)) provides the best graph data type currently implemented in C++. It is now a commercial product. You should at least study the methods it provides for graph manipulation, so as to see how the right level of abstract graph type makes implementing algorithms very clean and easy.

The C++ Boost Graph Library [SLL02] (*http://www.boost.org/libs/graph/doc*) is more readily available. Implementations of adjacency lists, matrices, and edge lists are included, along with a reasonable library of basic graph algorithms. Its interface and components are generic in the same sense as the C++ standard template library (STL).

JUNG (*http://jung.sourceforge.net/*) is a Java graph library particularly popular in the social networks community. The *Data Structures Library in Java* (JDSL) provides a comprehensive implementation with a decent algorithm library, and is available for noncommercial use at *http://www.jdsl.org/*. See [GTV05, GT05] for more detailed guides to JDSL. JGraphT (*http://jgrapht.sourceforge.net/*) is a more recent development with similar functionality.

The Stanford Graphbase (see Section 19.1.8 (page 660)) provides a simple but flexible graph data structure in CWEB, a literate version of the C language. It is instructive to see what Knuth does and does not place in his basic data structure, although we recommend other implementations as a better basis for further development.

My (biased) preference in C language graph types is the library from my book *Programming Challenges* [SR03]. See Section 19.1.10 (page 661) for details. Simple graph data structures in Mathematica are provided by *Combinatorica* [PS03], with a library of algorithms and display routines. See Section 19.1.9 (page 661).

Notes: The advantages of adjacency list data structures for graphs became apparent with the linear-time algorithms of Hopcroft and Tarjan [HT73b, Tar72]. The basic adjacency list and matrix data structures are presented in essentially all books on algorithms or data structures, including [CLRS01, AHU83, Tar83]. Hypergraphs are presented in Berge [Ber89]

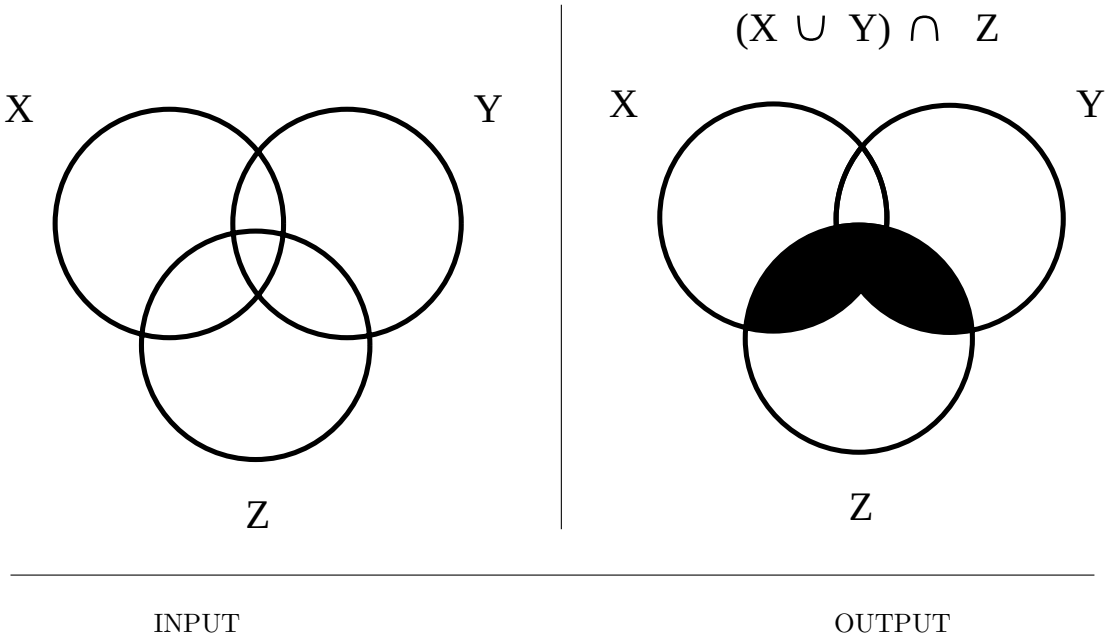
The improved efficiency of static graph types was revealed by Naher and Zlotowski [NZ02], who sped up certain LEDA graph algorithms by a factor of four by simply switching to a more compact graph structure.

An interesting question concerns minimizing the number of bits needed to represent arbitrary graphs on n vertices, particularly if certain operations must be supported efficiently. Such issues are surveyed in [vL90b].

Dynamic graph algorithms are data structures that maintain quick access to an invariant (such as minimum spanning tree or connectivity) under edge insertion and deletion. *Sparsification* [EGIN92] is a general approach to constructing dynamic graph algorithms. See [ACI92, Zar02] for experimental studies on the practicality of dynamic graph algorithms.

Hierarchically-defined graphs arise often in VLSI design problems, because designers make extensive use of cell libraries [Len90]. Algorithms specifically for hierarchically-defined graphs include planarity testing [Len89], connectivity [LW88], and minimum spanning trees [Len87a].

Related Problems: Set data structures (see page 385), graph partition (see page 541).



12.5 Set Data Structures

Input description: A universe of items $U = \{u_1, \ldots, u_n\}$ on which is defined a collection of subsets $S = \{S_1, \ldots, S_m\}$.

Problem description: Represent each subset so as to efficiently (1) test whether $u_i \in S_j$, (2) compute the union or intersection of S_i and S_j, and (3) insert or delete members of S.

Discussion: In mathematical terms, a set is an unordered collection of objects drawn from a fixed universal set. However, it is usually useful for implementation to represent each set in a single *canonical order*, typically sorted, to speed up or simplify various operations. Sorted order turns the problem of finding the union or intersection of two subsets into a linear-time operation—just sweep from left to right and see what you are missing. It makes possible element searching in sublinear time. Finally, printing the elements of a set in a canonical order paradoxically reminds us that order really doesn't matter.

We distinguish sets from two other kinds of objects: dictionaries and strings. A collection of objects *not* drawn from a fixed-size universal set is best thought of as a *dictionary*, discussed in Section 12.1 (page 367). Strings are structures where order matters—i.e. , if $\{A, B, C\}$ is not the same as $\{B, C, A\}$. Sections 12.3 and 18 discuss data structures and algorithms for strings.

Multisets permit elements to have more than one occurrence. Data structures for sets can generally be extended to multisets by maintaining a count field or linked list of equivalent entries for each element.

If each subset contains exactly two elements, they can be thought of as edges in a graph whose vertices represent the universal set. A system of subsets with no restrictions on the cardinality of its members is called a *hypergraph*. It is worth considering whether your problem has a graph-theoretical analogy, like connected components or shortest path in a graph/hypergraph.

Your primary alternatives for representing arbitrary subsets are:

- *Bit vectors* – An n-bit vector or array can represent any subset S on a universal set U containing n items. Bit i will be 1 if $i \in S$, and 0 if not. Since only one bit is needed per element, bit vectors can be very space efficient for surprisingly large values of $|U|$. Element insertion and deletion simply flips the appropriate bit. Intersection and union are done by "and-ing" or "or-ing" the bits together. The only drawback of a bit vector is its performance on sparse subsets. For example, it takes $O(n)$ time to explicitly identify all members of sparse (even empty) subset S.

- *Containers or dictionaries* – A subset can also be represented using a linked list, array, or dictionary containing exactly the elements in the subset. No notion of a fixed universal set is needed for such a data structure. For sparse subsets, dictionaries can be more space and time efficient than bit vectors, and easier to work with and program. For efficient union and intersection operations, it pays to keep the elements in each subset sorted, so a linear-time traversal through both subsets identifies all duplicates.

- *Bloom filters* – We can emulate a bit vector in the absence of a fixed universal set by hashing each subset element to an integer from 0 to n and setting the corresponding bit. Thus, bit $H(e)$ will be 1 if $e \in S$. Collisons leave some possibility for error under this scheme, however, because a different key might have hashed to the same position.

  Bloom filters use several (say k) different hash functions $H_1, \ldots H_k$, and set all k bits $H_i(e)$ upon insertion of key e. Now e is in S only if all k bits are 1. The probability of false positives can be made arbitrarily low by increasing the number of hash functions k and table size n. With the proper constants, each subset element can be represented using a constant number of bits independent of the size of the universal set.

  This hashing-based data structure is much more space-efficient than dictionaries for static subset applications that can tolerate a small probability of error. Many can. For instance, a spelling checker that left a rare random string undetected would prove no great tragedy.

Many applications involve collections of subsets that are pairwise disjoint, meaning that each element is in exactly one subset. For example, consider maintaining

the connected components of a graph or the party affiliations of politicians. Each vertex/hack is in exactly one component/party. Such a system of subsets is called a *set partition*. Algorithms for generating partitions of a given set are provided in Section 14.6 (page 456).

The primary issue with set partition data structures is maintaining changes over time, perhaps as edges are added or party members defect. Typical queries include "which set is a particular item in?" and "are two items in the same set?" as we modify the set by (1) changing one item, (2) merging or unioning two sets, or (3) breaking a set apart. Your basic options are:

- *Collection of containers* – Representing each subset in its own container/dictionary permits fast access to all the elements in the subset, which facilitates union and intersection operations. The cost comes in membership testing, as we must search each subset data structure independently until we find our target.

- *Generalized bit vector* – Let the ith element of an array denote the number/name of the subset that contains it. Set identification queries and single element modifications can be performed in constant time. However, operations like performing the union of two subsets take time proportional to the size of the universe, since each element in the two subsets must be identified and (at least one subset's worth) must have its name changed.

- *Dictionary with a subset attribute* – Similarly, each item in a binary tree can be associated a field that records the name of the subset it is in. Set identification queries and single element modifications can be performed in the time it takes to search in the dictionary. However, union/intersection operations are again slow. The need to perform such union operations quickly provides the motivation for the ...

- *Union-find data structure* – We represent a subset using a rooted tree where each node points to its *parent* instead of its children. The name of each subset will be the name of the item at the root. Finding out which subset we are in is simple, for we keep traversing up the parent pointers until we hit the root. Unioning two subsets is also easy. Just assign the root of one of two trees to point to the other, so now *all* elements have the same root and hence the same subset name.

  Implementation details have a big impact on asymptotic performance here. Always selecting the larger (or taller) tree as the root in a merger guarantees logarithmic height trees, as presented with our implementation in Section 6.1.3 (page 198). Retraversing the path traced on each find and explicitly pointing all nodes on the path to the root (called *path compression*) reduces the tree to almost constant height. Union find is a fast, simple data structure that every programmer should know about. It does not support breaking up subsets created by unions, but usually this is not an issue.

Implementations: Modern programming languages provide libraries offering complete and efficient set implementations. The C++ *Standard Template Library* (STL) provides `set` and `multiset` containers. *Java Collections* (JC) contains `HashSet` and `TreeSet` containers and is included in the `java.util` package of Java standard edition.

LEDA (see Section 19.1.1 (page 658)) provides efficient dictionary data structures, sparse arrays, and union-find data structures to maintain set partitions, all in C++.

Implementation of union-find underlies any implementation of Kruskal's minimum spanning tree algorithm. For this reason, all the graph libraries of Section 12.4 (page 381) presumably contains an implementation. Minimum spanning tree codes are described in Section 15.3 (page 484).

The computer algebra system *REDUCE* (*http://www.reduce-algebra.com/*) contains `SETS`, a package supporting set-theoretic operations on both explicit and implicit (symbolic) sets. Other computer algebra systems may support similar functionality.

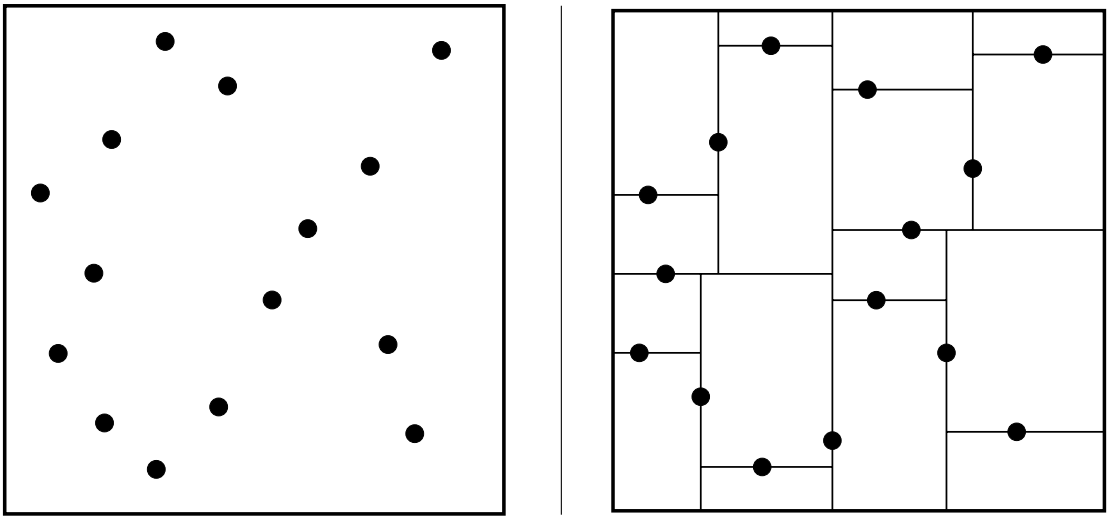
Notes: Optimal algorithms for such set operations as intersection and union were presented in [Rei72]. Raman [Ram05] provides an excellent survey on data structures for set operations on a variety of different operations. Bloom filters are ably surveyed in [BM05], with recent experimental results presented in [PSS07].

Certain balanced tree data structures support merge/meld/link/cut operations, which permit fast ways to union and intersect disjoint subsets. See Tarjan [Tar83] for a nice presentation of such structures. Jacobson [Jac89] augmented the bit-vector data structure to support select operations (where is the ith 1 bit?) efficiently in both time and space.

Galil and Italiano [GI91] survey data structures for disjoint set union. The upper bound of $O(m\alpha(m,n))$ on m union-find operations on an n-element set is due to Tarjan [Tar75], as is a matching lower bound on a restricted model of computation [Tar79]. The inverse Ackerman function $\alpha(m,n)$ grows notoriously slowly, so this performance is close to linear. An interesting connection between the worst-case of union-find and the length of Davenport-Schinzel sequences—a combinatorial structure that arises in computational geometry—is established in [SA95].

The *power set* of a set S is the collection of all $2^{|S|}$ subsets of S. Explicit manipulation of power sets quickly becomes intractable due to their size. Implicit representations of power sets in symbolic form becomes necessary for nontrivial computations. See [BCGR92] for algorithms on and computational experience with symbolic power set representations.

Related Problems: Generating subsets (see page 452), generating partitions (see page 456), set cover (see page 621), minimum spanning tree (see page 484).



INPUT OUTPUT

12.6 Kd-Trees

Input description: A set S of n points or more complicated geometric objects in k dimensions.

Problem description: Construct a tree that partitions space by half-planes such that each object is contained in its own box-shaped region.

Discussion: Kd-tree and related spatial data structures hierarchically decompose space into a small number of cells, each containing a few representatives from an input set of points. This provides a fast way to access any object by position. We traverse down the hierarchy until we find the smallest cell containing it, and then scan through the objects in this cell to identify the right one.

Typical algorithms construct kd-trees by partitioning point sets. Each node in the tree is defined by a plane cutting through one of the dimensions. Ideally, this plane equally partitions the subset of points into left/right (or up/down) subsets. These children are again partitioned into equal halves, using planes through a different dimension. Partitioning stops after $\lg n$ levels, with each point in its own leaf cell.

The cutting planes along any path from the root to another node defines a unique box-shaped region of space. Each subsequent plane cuts this box into two boxes. Each box-shaped region is defined by $2k$ planes, where k is the number of dimensions. Indeed, the "kd" in *kd-tree* is short for "k-dimensional." We maintain

the region of interest defined by the intersection of these half-spaces as we move down the tree.

Flavors of kd-trees differ in exactly how the splitting plane is selected. Options include:

- *Cycling through the dimensions* – partition first on d_1, then $d_2, \ldots, d_k$ before cycling back to d_1.
- *Cutting along the largest dimension* – select the partition dimension to make the resulting boxes as square or cube-like as possible. Selecting a plane to partition the points in half does not mean selecting a splitter in the middle of the box-shaped regions, since all the points may lie in the left side of the box.
- *Quadtrees or Octtrees* – Instead of partitioning with single planes, use all axis-parallel planes that pass through a given partition point. In two dimensions, this means creating four child cells; in 3D, this means eight child cells. Quadtrees seem particularly popular on image data, where leaf cells imply that all pixels in the regions have the same color.
- *BSP-trees – Binary space partitions* use general (i.e. , not just axis-parallel) cutting planes to carve up space into cells so that each cell ends up containing only one object (say a polygon). Such partitions are not possible using only axis-parallel cuts for certain sets of objects. The downside is that such polyhedral cell boundaries are more complicated to work with than boxes.
- *R-trees* – This is another spatial data structure useful for geometric objects that cannot be partitioned into axis-oriented boxes without cutting them into pieces. At each level, the objects are partitioned into a small number of (possibly-overlapping) boxes to construct searchable hierarchies without partitioning objects.

Ideally, our partitions split both the space (ensuring fat, regular regions) and the set of points (ensuring a log height tree) evenly, but doing both simultaneously can be impossible on a given input. The advantages of fat cells become clear in many applications of kd-trees:

- *Point location* – To identify which cell a query point q lies in, we start at the root and test which side of the partition plane contains q. By repeating this process on the appropriate child node, we travel down the tree to find the leaf cell containing q in time proportional to its height. See Section 17.7 (page 587) for more on point location.
- *Nearest neighbor search* – To find the point in S closest to a query point q, we perform point location to find the cell c containing q. Since c is bordered by some point p, we can compute the distance $d(p, q)$ from p to q. Point p is likely

close to q, but it might not be the single closest neighbor. Why? Suppose q lies right at the boundary of a cell. Then q's nearest neighbor might lie just to the left of the boundary in another cell. Thus, we must traverse all cells that lie within a distance of $d(p, q)$ of cell c and verify that none of them contain closer points. In trees with nice, fat cells, very few cells should need to be tested. See Section 17.5 (page 580) for more on nearest neighbor search.

- *Range search* – Which points lie within a query box or region? Starting from the root, check whether the query region intersects (or contains) the cell defining the current node. If it does, check the children; if not, none of the leaf cells below this node can possibly be of interest. We quickly prune away irrelevant portions of the space. Section 17.6 (page 584) focuses on range search.

- *Partial key search* – Suppose we want to find a point p in S, but we do not have full information about p. Say we are looking for someone of age 35 and height 5'8" but of unknown weight in a 3D-tree with dimensions of age, weight, and height. Starting from the root, we can identify the correct descendant for all but the weight dimension. To be sure we find the right point, we must search *both children* of these nodes. The more fields we know the better, but such partial key search can be substantially faster than checking all points against the key.

Kd-trees are most useful for a small to moderate number of dimensions, say from 2 up to maybe 20 dimensions. They lose effectiveness as the dimensionality increases, primarily because the ratio of the volume of a unit sphere in k-dimensions shrinks exponentially compared to the unit cube. Thus exponentially many cells will have to be searched within a given radius of a query point, say for nearest-neighbor search. Also, the number of neighbors for any cell grows to $2k$ and eventually become unmanageable.

The bottom line is that you should try to avoid working in high-dimensional spaces, perhaps by discarding (or projecting away) the least important dimensions.

Implementations: *KDTREE 2* contains C++ and Fortran 95 implementations of *kd*-trees for efficient nearest nearest neighbor search in many dimensions. See *http://arxiv.org/abs/physics/0408067*.

Samet's spatial index demos (*http://donar.umiacs.umd.edu/quadtree/*) provide a series of Java applets illustrating many variants of *kd*-trees, in association with his book [Sam06].

Terralib (*http://www.terralib.org/*) is an open source geographic information system (GIS) software library written in C++. This includes an implementation of spatial data structures.

The 1999 DIMACS implementation challenge focused on data structures for nearest neighbor search [GJM02]. Data sets and codes are accessible from *http://dimacs.rutgers.edu/Challenges*.

Notes: Samet [Sam06] is the best reference on kd-trees and other spatial data structures. All major (and many minor) variants are developed in substantial detail. A shorter survey [Sam05] is also available. Bentley [Ben75] is generally credited with developing kd-trees, although they have the murky history associated with most folk data structures.

The performance of spatial data structures degrades with high dimensionality. Projecting high-dimensional spaces onto a random lower-dimensional hyperplane has recently emerged as a simple but powerful method for dimensionality reduction. Both theoretical [IM04] and empirical [BM01] results indicate that this method preserves distances quite nicely.

Algorithms that quickly produce a point provably close to the query point are a recent development in higher-dimensional nearest neighbor search. A sparse weighted-graph structure is built from the data set, and the nearest neighbor is found by starting at a random point and walking greedily in the graph towards the query point. The closest point found during several random trials is declared the winner. Similar data structures hold promise for other problems in high-dimensional spaces. See [AM93, AMN$^+$98].

Related Problems: Nearest-neighbor search (see page 580), point location (see page 587), range search (see page 584).

13

Numerical Problems

If most problems you encounter are numerical in nature, there is an excellent chance that you are reading the wrong book. *Numerical Recipes* [PFTV07] gives a terrific overview to the fundamental problems in numerical computing, including linear algebra, numerical integration, statistics, and differential equations. Different flavors of the book include source code for all the algorithms in C++, Fortran, and even Pascal. Their coverage is somewhat skimpier on the combinatorial/numerical problems we consider in this section, but you should be aware of this book. Check it out at *http://www.nr.com*.

Numerical algorithms tend to be different beasts than combinatorial algorithms for at least two reasons:

- *Issues of Precision and Error* – Numerical algorithms typically perform repeated floating-point computations, which accumulate error at each operation until, eventually, the results are meaningless. My favorite example [MV99] concerns the Vancouver Stock Exchange, which over a twenty-two month period accumulated enough round-off error to reduce its index to 574.081 from the correct value of 1098.982.

  A simple and dependable way to test for round-off errors in numerical programs is to run them both at single and double precision, and then think hard whenever there is a disagreement.

- *Extensive Libraries of Codes* – Large, high-quality libraries of numerical routines have existed since the 1960s, which is still not yet the case for combinatorial algorithms. There are several reasons for this, including (1) the early emergence of Fortran as a standard for numerical computation, (2) the nature of numerical computations to be recognizably independent rather than

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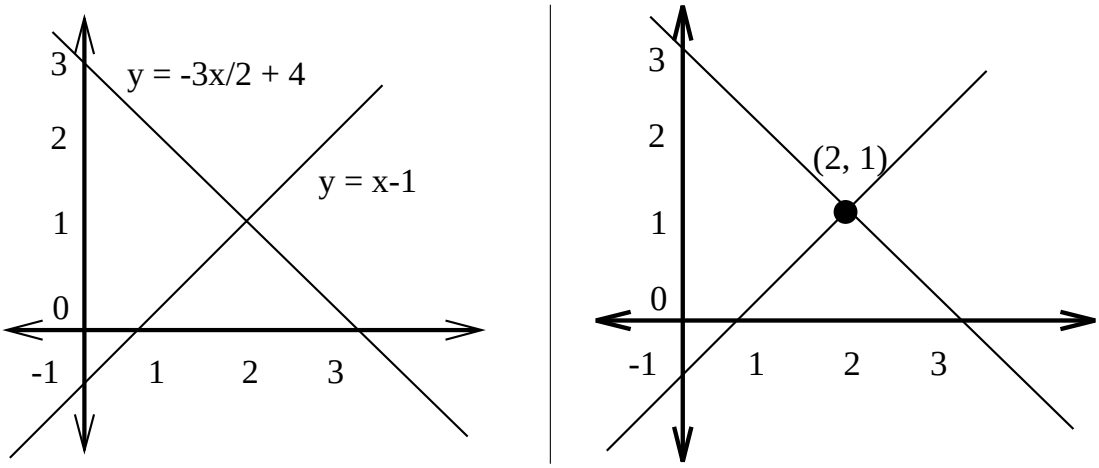
embedded within large applications, and (3) the existence of large scientific communities needing general numerical libraries.

Regardless of why, you should exploit this software base. There is probably no reason to implement algorithms for any of the problems in this section as opposed to using existing codes. Searching Netlib (see Section 19.1.5) is an excellent place to start.

Many scientist's and engineer's ideas about algorithms culturally derive from Fortran programming and numerical methods. Computer scientists grow up programming with pointers and recursion, and so are comfortable with the more sophisticated data structures required for combinatorial algorithms. Both sides can and should learn from each other, since problems such as pattern recognition can be modeled either numerically or combinatorially.

There is a vast literature on numerical algorithms. In addition to *Numerical Recipes*, recommended books include:

- *Chapara and Canale* [CC05] – The contemporary market leader in numerical analysis texts.
- *Mak* [Mak02] – This enjoyable text introduces Java to the world of numerical computation, and visa versa. Source code is provided.
- *Hamming* [Ham87] – This oldie but goodie provides a clear and lucid treatment of fundamental methods in numerical computation. It is available in a low-priced Dover edition.
- *Skeel and Keiper* [SK00] – A readable and interesting treatment of basic numerical methods, avoiding overly detailed algorithm descriptions through its use of the computer algebra system Mathematica. I like it.
- *Cheney and Kincaid* [CK07] – A traditional Fortran-based numerical analysis text, with discussions of optimization and Monte Carlo methods in addition to such standard topics as root-finding, numerical integration, linear systems, splines, and differential equations.
- *Buchanan and Turner* [BT92] – Thorough language-independent treatment of all standard topics, including parallel algorithms. It is the most comprehensive of the texts described here.



INPUT OUTPUT

13.1 Solving Linear Equations

Input description: An $m \times n$ matrix A and an $m \times 1$ vector b, together representing m linear equations on n variables.

Problem description: What is the vector x such that $A \cdot x = b$?

Discussion: The need to solve linear systems arises in an estimated 75% of all scientific computing problems [DB74]. For example, applying Kirchhoff's laws to analyze electrical circuits generates a system of equations—the solution of which puts currents through each branch of the circuit. Analysis of the forces acting on a mechanical truss generates a similar set of equations. Even finding the point of intersection between two or more lines reduces to solving a small linear system.

Not all systems of equations have solutions. Consider the equations $2x + 3y = 5$ and $2x + 3y = 6$. Some systems of equations have multiple solutions, such as $2x + 3y = 5$ and $4x + 6y = 10$. Such *degenerate* systems of equations are called *singular*, and they can be recognized by testing whether the determinant of the coefficient matrix is zero.

Solving linear systems is a problem of such scientific and commercial importance that excellent codes are readily available. There is no good reason to implement your own solver, even though the basic algorithm (Gaussian elimination) is one you learned in high school. This is especially true when working with large systems.

Gaussian elimination is based on the observation that the solution to a system of linear equations is invariant under scaling (if $x = y$, then $2x = 2y$) and adding

equations (the solution to $x = y$ and $w = z$ is the same as the solution to $x = y$ and $x + w = y + z$). Gaussian elimination scales and adds equations to eliminate each variable from all but one equation, leaving the system in such a state that the solution can be read off from the equations.

The time complexity of Gaussian elimination on an $n \times n$ system of equations is $O(n^3)$, since to clear the ith variable we add a scaled copy of the n-term ith row to each of the $n-1$ other equations. On this problem, however, constants matter. Algorithms that only partially reduce the coefficient matrix and then backsubstitute to get the answer use 50% fewer floating-point operations than the naive algorithm.

Issues to worry about include:

- *Are roundoff errors and numerical stability affecting my solution?* – Gaussian elimination would be quite straightforward to implement except for roundoff errors. These accumulate with each row operation and can quickly wreak havoc on the solution, particularly with matrices that are *almost* singular.

  To eliminate the danger of numerical errors, it pays to substitute the solution back into each of the original equations and test how close they are to the desired value. *Iterative methods* for solving linear systems refine initial solutions to obtain more accurate answers. Good linear systems packages will include such routines.

  The key to minimizing roundoff errors in Gaussian elimination is selecting the right equations and variables to pivot on, and to scale the equations to eliminate large coefficients. This is an art as much as a science, which is why you should use a well-crafted library routine as described next.

- *Which routine in the library should I use?* – Selecting the right code is also somewhat of an art. If you are taking your advice from this book, start with the general linear system solvers. Hopefully they will suffice for your needs. But search through the manual for more efficient procedures solving special types of linear systems. If your matrix happens to be one of these special types, the solution time can reduce from cubic to quadratic or even linear.

- *Is my system sparse?* – The key to recognizing that you have a special-case linear system is establishing how many matrix elements you really need to describe A. If there are only a few non-zero elements, your matrix is *sparse* and you are in luck. If these few non-zero elements are clustered near the diagonal, your matrix is *banded* and you are in even more luck. Algorithms for reducing the bandwidth of a matrix are discussed in Section 13.2. Many other regular patterns of sparse matrices can also be exploited, so consult the manual of your solver or a better book on numerical analysis for details.

- *Will I be solving many systems using the same coefficient matrix?* – In applications such as least-squares curve fitting, we must solve $A \cdot x = b$ repeatedly with different b vectors. We can preprocess A to make this easier. The lower-upper or *LU-decomposition* of A creates lower- and upper-triangular matrices

L and U such that $L \cdot U = A$. We can use this decomposition to solve $A \cdot x = b$, since

$$A \cdot x = (L \cdot U) \cdot x = L \cdot (U \cdot x) = b$$

This is efficient since backsubstitution solves a triangular system of equations in quadratic time. Solving $L \cdot y = b$ and then $U \cdot x = y$ gives the solution x using two $O(n^2)$ steps instead of one $O(n^3)$ step, after the LU-decomposition has been found in $O(n^3)$ time.

The problem of solving linear systems is equivalent to that of matrix inversion, since $Ax = B \leftrightarrow A^{-1}Ax = A^{-1}B$, where $I = A^{-1}A$ is the identity matrix. Avoid it however since matrix inversion proves to be three times slower than Gaussian elimination. LU-decomposition proves useful in inverting matrices as well as computing determinants (see Section 13.4 (page 404)).

Implementations: The library of choice for solving linear systems is apparently LAPACK—a descendant of LINPACK [DMBS79]. Both of these Fortran codes, as well as many others, are available from Netlib. See Section 19.1.5 (page 659).

Variants of LAPACK exist for other languages, like CLAPACK (C) and LAPACK++ (C++). The *Template Numerical Toolkit* is an interface to such routines in C++, and is available at *http://math.nist.gov/tnt/*.

JScience provides an extensive linear algebra package (including determinants) as part of its comprehensive scientific computing library. *JAMA* is another matrix package written in Java. Links to both and many related libraries are available at *http://math.nist.gov/javanumerics/*.

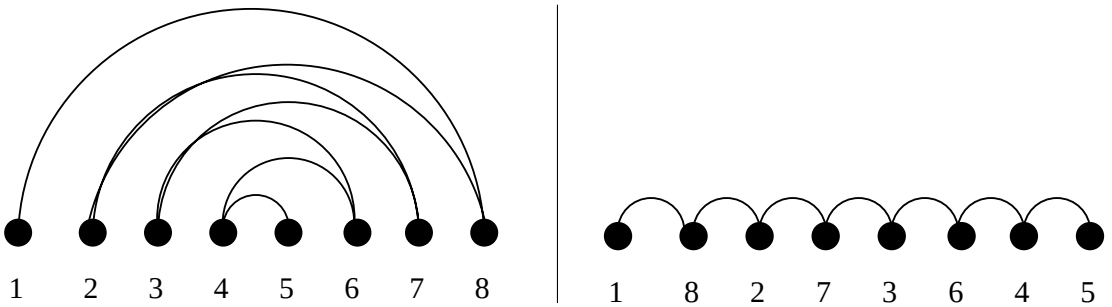
Numerical Recipes [PFTV07] (*www.nr.com*) provides guidance and routines for solving linear systems. Lack of confidence in dealing with numerical procedures is the most compelling reason to use these ahead of the free codes.

Notes: Golub and van Loan [GL96] is the standard reference on algorithms for linear systems. Good expositions on algorithms for Gaussian elimination and LU-decomposition include [CLRS01] and a host of numerical analysis texts [BT92, CK07, SK00]. Data structures for linear systems are surveyed in [PT05].

Parallel algorithms for linear systems are discussed in [Gal90, KSV97, Ort88]. Solving linear systems is one of most important applications where parallel architectures are used widely in practice.

Matrix inversion and (hence) linear systems solving can be done in matrix multiplication time using Strassen's algorithm plus a reduction. Good expositions on the equivalence of these problems include [AHU74, CLRS01].

Related Problems: Matrix multiplication (see page 401), determinant/permanent (see page 404).



13.2 Bandwidth Reduction

Input description: A graph $G = (V, E)$, representing an $n \times n$ matrix M of zero and non-zero elements.

Problem description: Which permutation p of the vertices minimizes the length of the longest edge when the vertices are ordered on a line—i.e. , minimizes $\max_{(i,j)\in E} |p(i) - p(j)|$?

Discussion: Bandwidth reduction lurks as a hidden but important problem for both graphs and matrices. Applied to matrices, bandwidth reduction permutes the rows and columns of a sparse matrix to minimize the distance b of any non-zero entry from the center diagonal. This is important in solving linear systems, because Gaussian elimination (see Section 13.1 (page 395)) can be performed in $O(nb^2)$ on matrices of bandwidth b. This is a big win over the general $O(n^3)$ algorithm if $b << n$.

Bandwidth minimization on graphs arises in more subtle ways. Arranging n circuit components in a line to minimize the length of the longest wire (and hence time delay) is a bandwidth problem, where each vertex of our graph corresponds to a circuit component and there is an edge for every wire linking two components. Alternatively, consider a hypertext application where we must store large objects (say images) on a magnetic tape. Each image has a set of possible images to visit next (i.e. , the hyperlinks). We seek to place linked images near each other on the tape to minimize the search time. This is exactly the bandwidth problem. More general formulations, such as rectangular circuit layouts and magnetic disks, inherit the same hardness and classes of heuristics from the linear versions.

The *bandwidth* problem seeks a linear ordering of the vertices, which minimizes the length of the longest edge, but there are several variations of the problem. In *linear arrangement*, we seek to minimize the sum of the lengths of the edges. This

has application to circuit layout, where we seek to position the chips to minimize the total wire length. In *profile minimization*, we seek to minimize the sum of one-way distances (i.e., for each vertex v) the length of the longest edge whose other vertex is to the left of of v.

Unfortunately, bandwidth minimization and all these variants is NP-complete. It stays NP-complete even if the input graph is a tree whose maximum vertex degree is 3, which is about as strong a condition as I have seen on any problem. Thus our only options are a brute-force search and heuristics.

Fortunately, ad hoc heuristics have been well studied and production-quality implementations of the best heuristics are available. These are based on performing a breadth-first search from a given vertex v, where v is placed at the leftmost point of the ordering. All of the vertices that are distance 1 from v are placed to its immediate right, followed by all the vertices at distance 2, and so forth until all vertices in G are accounted for. The popular heuristics differ according to how many different start vertices are considered and how equidistant vertices are ordered among themselves. Breaking ties with low-degree vertices over to the left however seems to be a good idea.

Implementations of the most popular heuristics—the Cuthill-McKee and Gibbs-Poole-Stockmeyer algorithms—are discussed in the implementation section. The worst case of the Gibbs-Poole-Stockmeyer algorithm is $O(n^3)$, which would wash out any possible savings in solving linear systems, but its performance in practice is close to linear.

Brute-force search programs can find the exact minimum bandwidth by backtracking through the set of $n!$ possible permutations of vertices. Considerable pruning can be achieved to reduce the search space by starting with a good heuristic bandwidth solution and alternately adding vertices to the left- and rightmost open slots in the partial permutation.

Implementations: Del Corso and Manzini's [CM99] code for exact solutions to bandwidth problems is available at *http://www.mfn.unipmn.it/∼manzini/bandmin*. Caprara and Salazar-González [CSG05] developed improved methods based on integer programming. Their branch-and-bound implementation in C is available at *http://joc.pubs.informs.org/Supplements/Caprara-2/*.

Fortran language implementations of both the Cuthill-McKee algorithm [CGPS76, Gib76, CM69] and the Gibbs-Poole-Stockmeyer algorithm [Lew82, GPS76] are available from Netlib. See Section 19.1.5 (page 659). Empirical evaluations of these and other algorithms on a test suite of 30 matrices are discussed in [Eve79b], showing Gibbs-Poole-Stockmeyer to be the consistent winner.

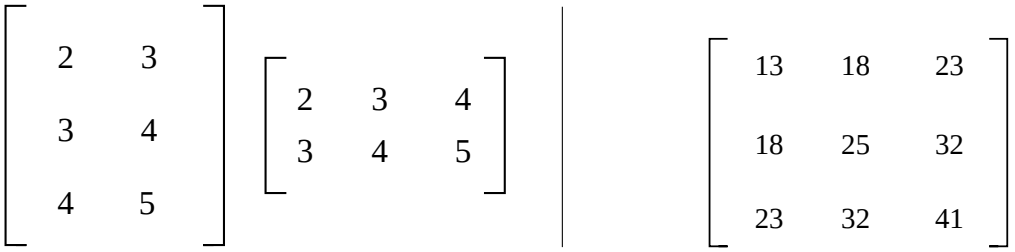
Petit [Pet03] performed an extensive experimental study on heuristics for the minimum linear arrangement problem. His codes and data are available at *http://www.lsi.upc.edu/∼jpetit/MinLA/Experiments/*.

Notes: Diaz et al. [DPS02] provide an excellent up-to-date survey on algorithms for bandwidth and related graph layout problems. See [CCDG82] for graph-theoretic and algorithmic results on bandwidth up to 1981.

Ad hoc heuristics have been widely studied—a tribute to its importance in numerical computation. Everstine [Eve79b] cites no less than 49 different bandwidth reduction algorithms! Del Corso and Romani [CR01] investigate a new class of spectral heuristics for bandwidth minimization.

The hardness of the bandwidth problem was first established by Papadimitriou [Pap76b], and its hardness on trees of maximum degree 3 in [GGJK78]. There are algorithms that run in polynomial time for fixed bandwidth k [Sax80]. Approximation algorithms offering a polylogarithmic guarantee exist for the general problem [BKRV00].

Related Problems: Solving linear equations (see page 395), topological sorting (see page 481).



13.3 Matrix Multiplication

Input description: An $x \times y$ matrix A and a $y \times z$ matrix B.

Problem description: Compute the $x \times z$ matrix $A \times B$.

Discussion: Matrix multiplication is a fundamental problem in linear algebra. Its main significance for combinatorial algorithms is its equivalence to many other problems, including transitive closure/reduction, parsing, solving linear systems, and matrix inversion. Thus, a faster algorithm for matrix multiplication implies faster algorithms for all of these problems. Matrix multiplication arises in its own right in computing the results of such coordinate transformations as scaling, rotation, and translation for robotics and computer graphics.

The following tight algorithm computes the product of $x \times y$ matrix A and $y \times z$ matrix B runs in $O(xyz)$. Remember to first initialize $M[i,j]$ to 0 for all $1 \leq i \leq x$ and $i \leq j \leq z$:

```
for i = 1 to x do
    for j = 1 to z
        for k = 1 to y
            M[i,j] = M[i,j] + A[i,k] · A[k,j]
```

An implementation in C appears in Section 2.5.4 (page 45). This straightforward algorithm would *seem* to be tough to beat in practice. That said, observe that the three loops can be arbitrarily permuted without changing the resulting answer. Such a permutation will change the memory access patterns and thus how effectively the cache memory is used. One can expect a 10-20% variation in run time among the six possible implementations, but could not confidently predict the winner (typically ikj) without running it on your machine with your given matrices.

When multiplying bandwidth-b matrices, where all non-zero elements of A and B lie within b elements of the main diagonals, a speedup to $O(xbz)$ is possible, since zero elements cannot contribute to the product.

Asymptotically faster algorithms for matrix multiplication exist, using clever divide-and-conquer recurrences. However, these prove difficult to program, require very large matrices to beat the trivial algorithm, and are less numerically stable to boot. The most famous of these is Strassen's $O(n^{2.81})$ algorithm. Empirical results (discussed next) disagree on the exact crossover point where Strassen's algorithm beats the simple cubic algorithm, but it is in the ballpark of $n \approx 100$.

There is a better way to save computation when you are multiplying a chain of more than two matrices together. Recall that multiplying an $x \times y$ matrix by a $y \times z$ matrix creates an $x \times z$ matrix. Thus, multiplying a chain of matrices from left to right might create large intermediate matrices, each taking a lot of time to compute. Matrix multiplication is not commutative, but it is associative, so we can parenthesize the chain in whatever manner we deem best without changing the final product. A standard dynamic programming algorithm can be used to construct the optimal parenthesization. Whether it pays to do this optimization will depend upon whether your matrix dimensions are sufficiently irregular and your chain multiplied often enough to justify it. Note that we are optimizing over the sizes of the dimensions in the chain, not the actual matrices themselves. No such optimization is possible if all your matrices are the same dimensions.

Matrix multiplication has a particularly interesting interpretation in counting the number of paths between two vertices in a graph. Let A be the adjacency matrix of a graph G, meaning $A[i,j] = 1$ if there is an edge between i and j. Otherwise, $A[i,j] = 0$. Now consider the square of this matrix, $A^2 = A \times A$. If $A^2[i,j] \geq 1$. This means that there must be a vertex k such that $A[i,k] = A[k,j] = 1$, so i to k to j is a path of length 2 in G. More generally, $A^k[i,j]$ counts the number of paths of length exactly k between i and j. This count includes nonsimple paths, where vertices are repeated, such as i to k to i to j.

Implementations: D'Alberto and Nicolau [DN07] have engineered a very efficient matrix multiplication code, which switches from Strassen's to the cubic algorithm at the optimal point. It is available at *http://www.ics.uci.edu/~fastmm/*. Earlier experiments put the crossover point where Strassen's algorithm beats the cubic algorithm at about $n = 128$ [BLS91, CR76].

Thus, an $O(n^3)$ algorithm will likely be your best bet unless your matrices are very large. The linear algebra library of choice is LAPACK, a descendant of LINPACK [DMBS79], which includes several routines for matrix multiplication. These Fortran codes are available from Netlib as discussed in Section 19.1.5 (page 659).

Algorithm 601 [McN83] of the Collected Algorithms of the ACM is a sparse matrix package written in Fortran that includes routines to multiply any combination of sparse and dense matrices. See Section 19.1.5 (page 659) for details.

Notes: Winograd's algorithm for fast matrix multiplication reduces the number of multiplications by a factor of two over the straightforward algorithm. It is implementable, although the additional bookkeeping required makes it doubtful whether it is a win. Expositions on Winograd's algorithm [Win68] include [CLRS01, Man89, Win80].

In my opinion, the history of theoretical algorithm design began when Strassen [Str69] published his $O(n^{2.81})$-time matrix multiplication algorithm. For the first time, improving an algorithm in the asymptotic sense became a respected goal in its own right. Progressive improvements to Strassen's algorithm have gotten progressively less practical. The current best result for matrix multiplication is Coppersmith and Winograd's [CW90] $O(n^{2.376})$ algorithm, while the conjecture is that $\Theta(n^2)$ suffices. See [CKSU05] for an alternate approach that recently yielded an $O(n^{2.41})$ algorithm.

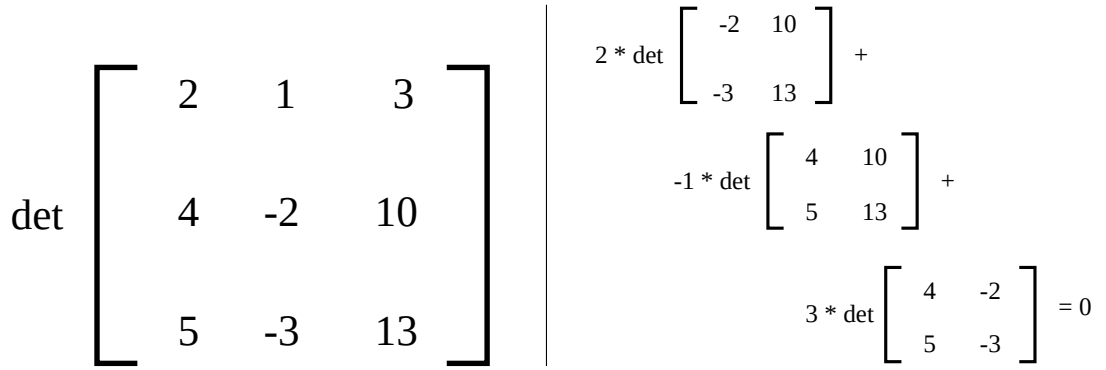
Engineering efficient matrix multiplication algorithms requires careful management of cache memory. See [BDN01, HUW02] for studies on these issues.

The interest in the squares of graphs goes beyond counting paths. Fleischner [Fle74] proved that the square of any biconnected graph has a Hamiltonian cycle. See [LS95] for results on finding the square roots of graphs—i.e. , finding A given A^2.

The problem of Boolean matrix multiplication can be reduced to that of general matrix multiplication [CLRS01]. The four-Russians algorithm for Boolean matrix multiplication [ADKF70] uses preprocessing to construct all subsets of $\lg n$ rows for fast retrieval in performing the actual multiplication, yielding a complexity of $O(n^3/\lg n)$. Additional preprocessing can improve this to $O(n^3/\lg^2 n)$ [Ryt85]. An exposition on the four-Russians algorithm, including this speedup, appears in [Man89].

Good expositions of the matrix-chain algorithm include [BvG99, CLRS01], where it is given as a standard textbook example of dynamic programming.

Related Problems: Solving linear equations (see page 395), shortest path (see page 489).



INPUT OUTPUT

13.4 Determinants and Permanents

Input description: An $n \times n$ matrix M.

Problem description: What is the determinant $|M|$ or permanent $perm(M)$ of the matrix m?

Discussion: Determinants of matrices provide a clean and useful abstraction in linear algebra that can be used to solve a variety of problems:

- Testing whether a matrix is *singular*, meaning that the matrix does not have an inverse. A matrix M is singular iff $|M| = 0$.
- Testing whether a set of d points lies on a plane in fewer than d dimensions. If so, the system of equations they define is singular, so $|M| = 0$.
- Testing whether a point lies to the left or right of a line or plane. This problem reduces to testing whether the sign of a determinant is positive or negative, as discussed in Section 17.1 (page 564).
- Computing the area or volume of a triangle, tetrahedron, or other simplicial complex. These quantities are a function of the magnitude of the determinant, as discussed in Section 17.1 (page 564).

The determinant of a matrix M is defined as a sum over all $n!$ possible permutations π_i of the n columns of M:

$$|M| = \sum_{i=1}^{n!} (-1)^{sign(\pi_i)} \prod_{j=1}^{n} M[j, \pi_j]$$

where $sign(\pi_i)$ denotes the number of pairs of elements out of order (called *inversions*) in permutation π_i.

A direct implementation of this definition yields an $O(n!)$ algorithm, as does the cofactor expansion method I learned in high school. Better algorithms to evaluate determinants are based on LU-decomposition, discussed in Section 13.1 (page 395). The determinant of M is simply the product of the diagonal elements of the LU-decomposition of M, which can be found in $O(n^3)$ time.

A closely related function called the *permanent* arises in combinatorial problems. For example, the permanent of the adjacency matrix of a graph G counts the number of perfect matchings in G. The permanent of a matrix M is defined by

$$perm(M) = \sum_{i=1}^{n!} \prod_{j=1}^{n} M[j, \pi_j]$$

differing from the determinant only in that all products are positive.

Surprisingly, it is NP-hard to compute the permanent, even though the determinant can easily be computed in $O(n^3)$ time. The fundamental difference is that $det(AB) = det(A) \times det(B)$, while $perm(AB) \neq perm(A) \times perm(B)$. There are permanent algorithms running in $O(n^2 2^n)$ time that prove to be considerably faster than the $O(n!)$ definition. Thus, finding the permanent of a 20×20 matrix is not out of the realm of possibility.

Implementations: The linear algebra package LINPACK contains a variety of Fortran routines for computing determinants, optimized for different data types and matrix structures. It can be obtained from Netlib, as discussed in Section 19.1.5 (page 659).

JScience provides an extensive linear algebra package (including determinants) as part of its comprehensive scientific computing library. *JAMA* is another matrix package written in Java. Links to both and many related libraries are available from *http://math.nist.gov/javanumerics/*.

Nijenhuis and Wilf [NW78] provide an efficient Fortran routine to compute the permanent of a matrix. See Section 19.1.10 (page 661). Cash [Cas95] provides a C routine to compute the permanent, motivated by the Kekulé structure count of computational chemistry.

Two different codes for approximating the permanent are provided by Barvinok. The first, based on [BS07], provides codes for approximating the permanent and a Hafnian of a matrix, as well as the number of spanning forests in a graph. See *http://www.math.lsa.umich.edu/∼barvinok/manual.html*. The second, based on [SB01], can provide estimates of the permanent of 200×200 matrices in seconds. See *http://www.math.lsa.umich.edu/∼barvinok/code.html*.

Notes: Cramer's rule reduces the problems of matrix inversion and solving linear systems to that of computing determinants. However, algorithms based on LU-determination are faster. See [BM53] for an exposition on Cramer's rule.

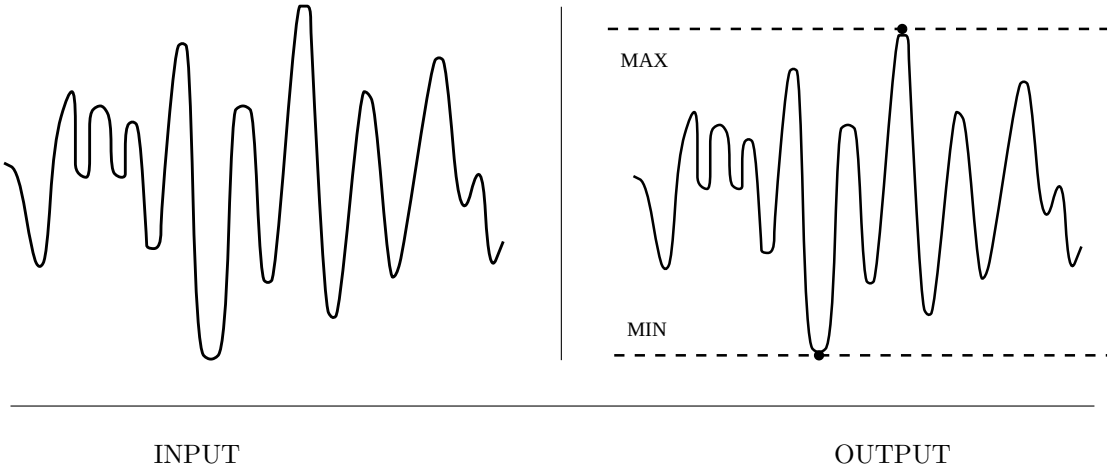
Determinants can be computed in $o(n^3)$ time using fast matrix multiplication, as shown in [AHU83]. Section 13.3 (page 401) discusses such algorithms. A fast algorithm for computing the sign of the determinant—an important problem for performing robust geometric computations—is due to Clarkson [Cla92].

The problem of computing the permanent was shown to be #P-complete by Valiant [Val79], where #P is the class of problems solvable on a "counting" machine in polynomial time. A counting machine returns the number of distinct solutions to a problem. Counting the number of Hamiltonian cycles in a graph is a #P-complete problem that is trivially NP-hard (and presumably harder), since any count greater than zero proves that the graph is Hamiltonian. Counting problems can be #P-complete even if the corresponding decision problem can be solved in polynomial time, as shown by the permanent and perfect matchings.

Minc [Min78] is the primary reference on permanents. A variant of an $O(n^2 2^n)$-time algorithm due to Ryser for computing the permanent is presented in [NW78].

Recently, probabilistic algorithms have been developed for estimating the permanent, culminating in a fully-polynomial randomized approximation scheme that provides an arbitrary close approximation in time that depends polynomially upon the input matrix and the desired error [JSV01].

Related Problems: Solving linear systems (see page 395), matching (see page 498), geometric primitives (see page 564).



13.5 Constrained and Unconstrained Optimization

Input description: A function $f(x_1, \ldots, x_n)$.

Problem description: What point $p = (p_1, \ldots, p_n)$ maximizes (or minimizes) the function f?

Discussion: Most of this book concerns algorithms that optimize one thing or another. This section considers the general problem of optimizing functions where, due to lack of structure or knowledge, we are unable to exploit the problem-specific algorithms seen elsewhere in this book.

Optimization arises whenever there is an objective function that must be tuned for optimal performance. Suppose we are building a program to identify good stocks to invest in. We have certain financial data available to analyze—such as the price-earnings ratio, the interest rate, and the stock price—all as a function of time t. The key question is how much weight we should give to each of these factors, where these weights correspond to coefficients of a formula:

$$\text{stock-goodness}(t) = c_1 \times \text{price}(t) + c_2 \times \text{interest}(t) + c_3 \times \text{PE-ratio}(t)$$

We seek the numerical values c_1, c_2, c_3 whose stock-goodness function does the best job of evaluating stocks. Similar issues arise in tuning evaluation functions for any pattern recognition task.

Unconstrained optimization problems also arise in scientific computation. Physical systems from protein structures to galaxies naturally seek to minimize their "energy" or "potential function." Programs that attempt to simulate nature thus often define potential functions assigning a score to each possible object configuration, and then select the configuration that minimizes this potential.

Global optimization problems tend to be hard, and there are lots of ways to go about them. Ask the following questions to steer yourself in the right direction:

- *Am I doing constrained or unconstrained optimization?* – In unconstrained optimization, there are no limitations on the values of the parameters other than that they maximize the value of f. However, many applications demand constraints on these parameters that make certain points illegal, points that might otherwise be the global optimum. For example, companies cannot employ less than zero employees, no matter how much money they think they might save doing so. Constrained optimization problems typically require mathematical programming approaches, like linear programming, discussed in Section 13.6 (page 411).

- *Is the function I am trying to optimize described by a formula?* – Sometimes the function that you seek to optimize is presented as an algebraic formula, such as finding the minimum of $f(n) = n^2 - 6n + 2^{n+1}$. If so, the solution is to analytically take its derivative $f'(n)$ and see for which points p' we have $f'(p') = 0$. These points are either local maxima or minima, which can be distinguished by taking a second derivative or just plugging p' back into f and seeing what happens. Symbolic computation systems such as Mathematica and Maple are fairly effective at computing such derivatives, although using computer algebra systems effectively is somewhat of a black art. They are definitely worth a try, however, and you can always use them to plot a picture of your function to get a better idea of what you are dealing with.

- *Is it expensive to compute the function at a given point?* – Instead of a formula, we are often given a program or subroutine that evaluates f at a given point. Since we can request the value of any given point on demand by calling this function, we can poke around and try to guess the maxima.

  Our freedom to search in such a situation depends upon how efficiently we can evaluate f. Suppose that $f\ (x_1, \ldots, x_n)$ is the board evaluation function in a computer chess program, such that x_1 is how much a pawn is worth, x_2 is how much a bishop is worth, and so forth. To evaluate a set of coefficients as a board evaluator, we must play a bunch of games with it or test it on a library of known positions. Clearly, this is time-consuming, so we would have to be frugal in the number of evaluations of f we use to optimize the coefficients.

- *How many dimensions do we have? How many do we need?* – The difficulty in finding a global maximum increases rapidly with the number of dimensions (or parameters). For this reason, it often pays to reduce the dimension by ignoring some of the parameters. This runs counter to intuition, for the naive programmer is likely to incorporate as many variables as possible into their evaluation function. It is just too hard, however, to optimize such complicated

functions. Much better is to start with the three to five most important variables and do a good job optimizing the coefficients for these.

- *How smooth is my function?* The main difficulty of global optimization is getting trapped in local optima. Consider the problem of finding the highest point in a mountain range. If there is only one mountain and it is nicely shaped, we can find the top by just walking in whatever direction is up. However, if there are many false summits, or other mountains in the area, it is difficult to convince ourselves whether we really are at the highest point. *Smoothness* is the property that enables us to quickly find the local optimum from a given point. We assume smoothness in seeking the peak of the mountain by walking up. If the height at any given point was a completely random function, there would be no way we could find the optimum height short of sampling every single point.

The most efficient algorithms for unconstrained global optimization use derivatives and partial derivatives to find local optima, to point out the direction in which moving from the current point does the most to increase or decrease the function. Such derivatives can sometimes be computed analytically, or they can be estimated numerically by taking the difference between the values of nearby points. A variety of *steepest descent* and *conjugate gradient* methods to find local optima have been developed—similar in many ways to numerical root-finding algorithms.

It is a good idea to try several different methods on any given optimization problem. For this reason, we recommend experimenting with the implementations below before attempting to implement your own method. Clear descriptions of these algorithms are provided in several numerical algorithms books, in particular *Numerical Recipes* [PFTV07].

For constrained optimization, finding a point that satisfies all the constraints is often the difficult part of the problem. One approach is to use a method for unconstrained optimization, but add a penalty according to how many constraints are violated. Determining the right penalty function is problem-specific, but it often makes sense to vary the penalties as optimization proceeds. At the end, the penalties should be very high to ensure that all constraints are satisfied.

Simulated annealing is a fairly robust and simple approach to constrained optimization, particularly when we are optimizing over combinatorial structures (permutations, graphs, subsets). Techniques for simulated annealing are described in Section 7.5.3 (page 254).

Implementations: The world of constrained/unconstrained optimization is sufficiently confusing that several guides have been created to point people to the right codes. Particularly nice is Hans Mittlemann's *Decision Tree for Optimization Software* at *http://plato.asu.edu/guide.html*. Also check out the selection at GAMS, the NIST *Guide to Available Mathematical Software*, at http://gams.nist.gov.

NEOS (Network-Enabled Optimization System) provides a unique service—the opportunity to solve your problem remotely on computers and software at Argonne

National Laboratory. Linear programming and unconstrained optimization are both supported. Check out *http://www-neos.mcs.anl.gov/* when you need a solution instead of a program.

Several of the *Collected Algorithms of the ACM* are Fortran codes for unconstrained optimization, most notably Algorithm 566 [MGH81] , Algorithm 702 [SF92] , and Algorithm 734 [Buc94] . Algorithm 744 [Rab95] does unconstrained optimization in Lisp. They are all available from Netlib (see Section 19.1.5 (page 659)).

General purpose simulated annealing implementations are available, and probably are the best place to start experimenting with this technique for constrained optimization. Feel free to try my code from Section 7.5.3 (page 254). Particularly popular is *Adaptive Simulated Annealing (ASA)*, written in C by Lester Ingber and available at *http://asa-caltech.sourceforge.net/*.

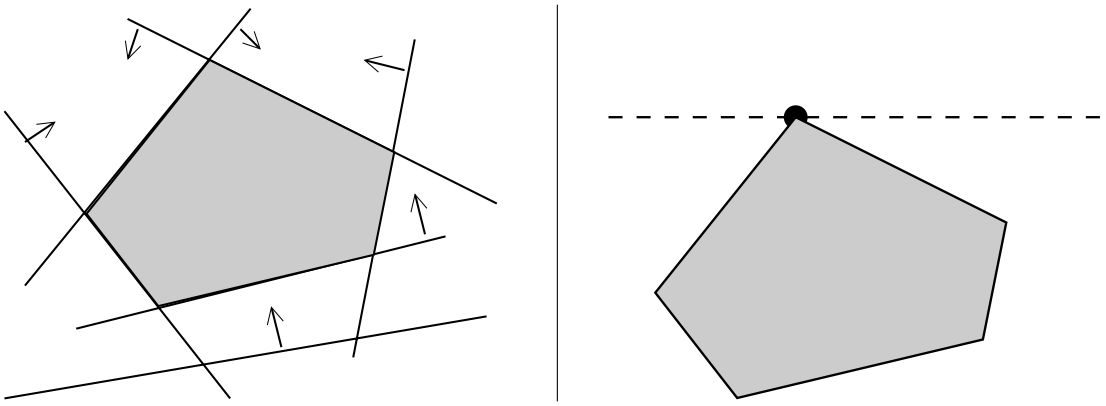
Both the Java Genetic Algorithms Package (JGAP) (*http://jgap.sourceforge.net/*) and the C Genetic Algorithm Utility Library (GAUL) (*http://gaul.sourceforge.net/*) are designed to aid in the development of applications that use genetic/evolutionary algorithms. I am highly skeptical about genetic algorithms (see Section 7.8 (page 266)), but other people seem to find them irresistible.

Notes: Steepest-descent methods for unconstrained optimization are discussed in most books on numerical methods, including [BT92, PFTV07]. Unconstrained optimization is the topic of several books, including [Bre73, Fle80].

Simulated annealing was devised by Kirkpatrick et al. [KGV83] as a modern variation of the Metropolis algorithm [MRRT53]. Both use Monte Carlo techniques to compute the minimum energy state of a system. Good expositions on all local search variations, including simulated annealing, appear in [AL97].

Genetic algorithms were developed and popularized by Holland [Hol75, Hol92]. More sympathetic expositions on genetic algorithms include [LP02, MF00]. Tabu search [Glo90] is yet another heuristic search procedure with a devoted following.

Related Problems: Linear programming (see page 411), satisfiability (see page 472).



INPUT OUTPUT

13.6 Linear Programming

Input description: A set S of n linear inequalities on m variables

$$S_i := \sum_{j=1}^{m} c_{ij} \cdot x_j \geq b_i,\ 1 \leq i \leq n$$

and a linear optimization function $f(X) = \sum_{j=1}^{m} c_j \cdot x_j$.

Problem description: Which variable assignment X' maximizes the objective function f while satisfying all inequalities S?

Discussion: Linear programming is the most important problem in mathematical optimization and operations research. Applications include:

- *Resource allocation* – We seek to invest a given amount of money to maximize our return. Often our possible options, payoffs, and expenses can be expressed as a system of linear inequalities such that we seek to maximize our possible profit given the constraints. Very large linear programming problems are routinely solved by airlines and other corporations.
- *Approximating the solution of inconsistent equations* – A set of m linear equations on n variables x_i, $1 \leq i \leq n$ is overdetermined if $m > n$. Such overdetermined systems are often *inconsistent*, meaning that there does not exist an assignment to the variables that simultaneously solves all the equations. To find the assignment that best fits the equations, we can replace each variable x_i by $x'_i + \epsilon_i$ and solve the new system as a linear program, minimizing the sum of the error terms.

- *Graph algorithms* – Many of the graph problems described in this book, including shortest path, bipartite matching, and network flow, can be solved as special cases of linear programming. Most of the rest, including traveling salesman, set cover, and knapsack, can be solved using *integer linear programming*.

The *simplex method* is the standard algorithm for linear programming. Each constraint in a linear programming problem acts like a knife that carves away a region from the space of possible solutions. We seek the point within the remaining region that maximizes (or minimizes) $f(X)$. By appropriately rotating the solution space, the optimal point can always be made to be the highest point in the region. The region (simplex) formed by the intersection of a set of linear constraints is convex, so unless we are at the top there is always a higher vertex neighboring any starting point. When we cannot find a higher neighbor to walk to, we have reached the optimal solution.

While the simplex algorithm is not too complex, there is considerable art to producing an efficient implementation capable of solving large linear programs. Large programs tend to be sparse (meaning that most inequalities use few variables), so sophisticated data structures must be used. There are issues of numerical stability and robustness, as well as choosing which neighbor we should walk to next (so-called *pivoting rules*). There also exist sophisticated *interior-point* methods, which cut through the interior of the simplex instead of walking along the outside, and beat simplex in many applications.

The bottom line on linear programming is this: you are much better off using an existing LP code than writing your own. Further, you are probably better off paying money than surfing the Web. Linear programming is an algorithmic problem of such economic importance that commercial implementations are far superior to free versions.

Issues that arise in linear programming include:

- *Do any variables have integrality constraints?* – It is impossible to send 6.54 airplanes from New York to Washington each business day, even if that value maximizes profit according to your model. Such variables often have natural integrality constraints. A linear program is called an *integer program* if all its variables have integrality constraints, or a *mixed integer program* if some of them do.

  Unfortunately, it is NP-complete to solve integer or mixed programs to optimality. However, there are integer programming techniques that work reasonably well in practice. *Cutting plane techniques* solve the problem first as a linear program, and then add extra constraints to enforce integrality around the optimal solution point before solving it again. After sufficiently many iterations, the optimum point of the resulting linear program matches that of the original integer program. As with most exponential-time algorithms,

run times for integer programming depend upon the difficulty of the problem instance and are unpredictable.

- *Do I have more variables or constraints?* – Any linear program with m variables and n inequalities can be written as an equivalent *dual* linear program with n variables and m inequalities. This is important to know, because the running time of a solver might be quite different on the two formulations. In general, linear programs (LPs) with much more variables than constraints should be solved directly. If there are many more constraints than variables, it is usually better to solve the dual LP or (equivalently) apply the dual simplex method to the primal LP.

- *What if my optimization function or constraints are not linear?* – In least-squares curve fitting, we seek the line that best approximates a set of points by minimizing the sum of squares of the distance between each point and the line. In formulating this as a mathematical program, the natural objective function is no longer linear, but quadratic. Although fast algorithms exist for least squares fitting, general *quadratic programming* is NP-complete.

  There are three possible courses of action when you must solve a nonlinear program. The best is if you can model it in some other way, as is the case with least-squares fitting. The second is to try to track down special codes for quadratic programming. Finally, you can model your problem as a constrained or unconstrained optimization problem and try to solve it with the codes discussed in Section 13.5 (page 407).

- *What if my model does not match the input format of my LP solver?* – Many linear programming implementations accept models only in so-called *standard form*, where all variables are constrained to be nonnegative, the object function must be minimized, and all constraints must be equalities (instead of inequalities).

  Do not fear. There exist standard transformations to map arbitrary LP models into standard form. To convert a maximization problem to a minimization one, simply multiply each coefficient of the objective function by -1. The remaining problems can be solved by adding *slack variables* to the model. See any textbook on linear programming for details. Modeling languages such as AMPC can provide a nice interface to your solver and deal with these issues for you.

Implementations: The USENET Frequently Asked Question (FAQ) list is a very useful resource on solving linear programs. In particular, it provides a list of available codes with descriptions of experiences. Check it out at *http://www-unix.mcs.anl.gov/otc/Guide/faq/*.

There are at least three reasonable choices in free LP-solvers. `Lp_solve`, written in ANSI C by Michel Berkelaar, can also handle integer and mixed-integer

problems. It is available at *http://lpsolve.sourceforge.net/5.5/*, and a substantial user community exists. The simplex solver `CLP` produced under the Computational Infrastructure for Operations Research is available (with other optimization software) at *http://www.coin-or.org/*. Finally, the GNU Linear Programming Kit (GLPK) is intended for solving large-scale linear programming, mixed integer programming (MIP), and other related problems. It is available at *http://www.gnu.org/software/glpk/*. In recent benchmarks among free codes (see *http://plato.asu.edu/bench.html*), `CLP` appeared to be fastest on on linear programming problems and `lp_solve` on mixed integer problems.

NEOS (Network-Enabled Optimization System) provides an opportunity to solve your problem on computers and software at Argonne National Laboratory. Linear programming and unconstrained optimization are both supported. This is worth checking out at *http://www.mcs.anl.gov/home/otc/Server/* if you need an answer instead of a program.

Algorithm 551 [Abd80] and Algorithm 552 [BR80] of the *Collected Algorithms of the ACM* are simplex-based codes for solving overdetermined systems of linear equations in Fortran. See Section 19.1.5 (page 659) for details.

Notes: The need for optimization via linear programming arose in logistics problems in World War II. The simplex algorithm was invented by George Danzig in 1947 [Dan63]. Klee and Minty [KM72] proved that the simplex algorithm is exponential in worst case, but it is very efficient in practice.

Smoothed analysis measures the complexity of algorithms assuming that their inputs are subject to small amounts of random noise. Carefully constructed worst-case instances for many problems break down under such perturbations. Spielman and Teng [ST04] used smoothed analysis to explain the efficiency of simplex in practice. Recently, Kelner and Spielman developed a randomized simplex algorithm running in polynomial time [KS05b].

Khachian's ellipsoid algorithm [Kha79] first proved that linear programming was polynomial in 1979. Karmarkar's algorithm [Kar84] is an interior-point method that has proven to be both a theoretical and practical improvement of the ellipsoid algorithm, as well as a challenge for the simplex method. Good expositions on the simplex and ellipsoid algorithms for linear programming include [Chv83, Gas03, MG06].

Semidefinite programming deals with optimization problems over symmetric positive semidefinite matrix variables, with linear cost function and linear constraints. Important special cases include linear programming and convex quadratic programming with convex quadratic constraints. Semidefinite programming and its applications to combinatorial optimization problems are surveyed in [Goe97, VB96].

Linear programming is P-complete under log-space reductions [DLR79]. This makes it unlikely to have an NC parallel algorithm, where a problem is in NC iff it can be solved on a PRAM in polylogarithmic time using a polynomial number of processors. Any problem that is P-complete under log-space reduction cannot be in NC unless P=NC. See [GHR95] for a thorough exposition of the theory of P-completeness, including an extensive list of P-complete problems.

Related Problems: Constrained and unconstrained optimization (see page 407), network flow (see page 509).

13.7 Random Number Generation

Input description: Nothing, or perhaps a seed.

Problem description: Generate a sequence of random integers.

Discussion: Random numbers have an enormous variety of interesting and important applications. They form the foundation of simulated annealing and related heuristic optimization techniques. Discrete event simulations run on streams of random numbers, and are used to model everything from transportation systems to casino poker. Passwords and cryptographic keys are typically generated randomly. Randomized algorithms for graph and geometric problems are revolutionizing these fields and establishing randomization as one of the fundamental ideas of computer science.

Unfortunately, generating random numbers looks a lot easier than it really is. Indeed, it is fundamentally impossible to produce truly random numbers on any deterministic device. Von Neumann [Neu63] said it best: "Anyone who considers arithmetical methods of producing random digits is, of course, in a state of sin." The best we can hope for are *pseudorandom* numbers, a stream of numbers that appear as if they were generated randomly.

There can be serious consequences to using a bad random-number generator. In one famous case, a Web browser's encryption scheme was broken with the discovery that the seeds of its random-number generator employed too few random bits [GW96]. Simulation accuracy is regularly compromised or invalidated by poor random number generation. This is an area where people shouldn't mess around, but they do. Issues to think about include:

- *Should my program use the same "random" numbers each time it runs?* – A poker game that deals you the exact same hand each time you play quickly loses interest. One common solution is to use the lower-order bits of the machine clock as the *seed* or starting point for a stream of random numbers, so that each time the program runs it does something different.

Such methods are adequate for games, but not for serious simulations. There are liable to be periodicities in the distribution of random numbers whenever calls are made in a loop. Also, debugging is seriously complicated when program results are not repeatable. Should your program crash, you cannot go back and discover why. A possible compromise is to use a deterministic pseudorandom-number generator, but write the current seed to a file between runs. During debugging, this file can be overwritten with a fixed initial value of the seed.

- *How good is my compiler's built-in random number generator?* – If you need uniformly-generated random numbers, and won't be betting the farm on the accuracy of your simulation, my recommendation is simply to use what your compiler provides. Your best opportunity to mess things up is with a bad choice of starting seed, so read the manual for its recommendations.

  If you *are* going to bet the farm on the results of your simulation, you had better test your random number generator. Be aware that it is very difficult to eyeball the results and decide whether the output is really random. This is because people have very skewed ideas of how random sources should behave and often see patterns that don't really exist. Several different tests should be used to evaluate a random number generator, and the statistical significance of the results established. The National Institute of Standards and Technology (NIST) has developed a test suite for evaluating random number generators, discussed below.

- *What if I must implement my own random-number generator?* – The standard algorithm of choice is the *linear congruential generator*. It is fast, simple, and (if instantiated with the right constants) gives reasonable pseudorandom numbers. The nth random number R_n is a function of the $(n-1)$st random number:

  $$R_n = (aR_{n-1} + c) \bmod m$$

  In theory, linear congruential generators work the same way roulette wheels do. The long path of the ball around and around the wheel (captured by $aR_{n-1} + c$) ends in one of a relatively small number of bins, the choice of which is extremely sensitive to the length of the path (captured by the mod m-truncation).

  A substantial theory has been developed to select the constants a, c, m, and R_0. The period length is largely a function of the modulus m, which is typically constrained by the word length of the machine.

  Note that the stream of numbers produced by a linear congruential generator repeats the instant the first number repeats. Further, computers are fast enough to make 2^{32} calls to a random-number generator in a few minutes. Thus, any 32-bit linear congruential generator is in danger of cycling, motivating generators with significantly longer periods.

- *What if I don't want such large random numbers?* – The linear congruential generator produces a uniformly-distributed sequence of large integers that can be easily scaled to produce other uniform distributions. For uniformly distributed real numbers between 0 and 1, use R_i/m. Note that 1 cannot be realized this way, although 0 can. If you want uniformly distributed integers between l and h, use $\lfloor l + (h - l + 1)R_i/m \rfloor$.

- *What if I need nonuniformly distributed random numbers?* – Generating random numbers according to a given nonuniform distribution can be a tricky business. The most reliable way to do this correctly is the acceptance-rejection method. We can bound the desired geometric region to sample from by a box and then select a random point p from the box. This point can be generated by selecting the x and y coordinates independently at random. If it lies within the region of interest, we can return p as being selected at random. Otherwise we throw it away and repeat with another random point. Essentially, we throw darts at random and report those that hit the target.

  This method is correct, but it can be slow. If the volume of the region of interest is small relative to that of the box, most of our darts will miss the target. Efficient generators for Gaussian and other special distributions are described in the references and implementations below.

  Be cautious about inventing your own technique, however, since it can be tricky to obtain the right probability distribution. For example, an *incorrect* way to select points uniformly from a circle of radius r would be to generate polar coordinates by selecting an angle from 0 to 2π and a displacement between 0 and r—both uniformly at random. In such a scheme, half the generated points will lie within $r/2$ of the center, when only one-fourth of them should be! This is different enough to seriously skew the results, while being sufficiently subtle that it can easily escape detection.

- *How long should I run my Monte Carlo simulation to get the best results?* – The longer you run a simulation, the more accurately the results should approximate the limiting distribution, thus increasing accuracy. However, this is true only until you exceed the *period*, or cycle length, of your random-number generator. At that point, your sequence of random numbers repeats itself, and further runs generate no additional information.

  Instead of jacking up the length of a simulation run to the max, it is usually more informative to do many shorter runs (say 10 to 100) with different seeds and then consider the range of results you see. The variance provides a healthy measure of the degree to which your results are repeatable. This exercise corrects the natural tendency to see a simulation as giving "the" correct answer.

Implementations: See *http://random.mat.sbg.ac.at* for an excellent website on random-number generation and stochastic simulation. It includes pointers to papers and literally dozens of implementations of random-number generators.

Parallel simulations make special demands on random-number generators. How can we ensure that random streams are independent on each machine? L'Ecuyer et.al. [LSCK02] provide object-oriented generators with a period length of approximately 2^{191}. Implementations in C, C++, and Java are available at *http://www.iro.umontreal.ca/~lecuyer/myftp/streams00/*. Independent streams of random numbers are supported for parallel applications. Another possibility is the *Scalable Parallel Random Number Generators Library (SPRNG)* [MS00], available at *http://sprng.cs.fsu.edu/*.

Algorithms 488 [Bre74], 599 [AKD83], and 712 [Lev92] of the *Collected Algorithms of the ACM* are Fortran codes for generating non-uniform random numbers according to several probability distributions, including the normal, exponential, and Poisson distributions. They are available from Netlib (see Section 19.1.5 (page 659)).

The National Institute of Standards [RSN+01] has prepared an extensive statistical test suite to validate random number generators. Both the software and the report describing it are available at *http://csrc.nist.gov/rng/*.

True random-number generators extract random bits by observing physical processes. The website *http://www.random.org* makes available random numbers derived from atmospheric noise that passes the NIST statistical tests. This is an amusing solution if you need a small quantity of random numbers (say, to run a lottery) instead a random-number generator.

Notes: Knuth [Knu97b] provides a thorough treatment of random-number generation, which I heartily recommend. He presents the theory behind several methods, including the middle-square and shift-register methods we have not described here, as well as a detailed discussion of statistical tests for validating random-number generators.

That said, see [Gen04] for more recent developments in random number generation. The Mersenne twister [MN98] is a fast random number generator of period $2^{19937} - 1$. Other modern methods include [Den05, PLM06]. Methods for generating nonuniform random variates are surveyed in [HLD04]. Comparisons of different random-number generators in practice include [PM88].

Tables of random numbers appear in most mathematical handbooks as relics from the days before there was ready access to computers. Most notable is [RC55], which provides one million random digits.

The deep relationship between randomness, information, and compressibility is explored within the theory of Kolmogorov complexity, which measures the complexity of a string by its compressibility. Truly random strings are incompressible. The string of seemingly random digits of π cannot be random under this definition, since the entire sequence is defined by any program implementing a series expansion for π. Li and Vitáni [LV97] provide a thorough introduction to the theory of Kolmogorov complexity.

Related Problems: Constrained and unconstrained optimization (see page 407), generating permutations (see page 448), generating subsets (see page 452), generating partitions (see page 456).

833816926455584605284210207 1	179424673 2038074743 * 22801763489 --- 833816926455584605284210207 1

INPUT OUTPUT

13.8 Factoring and Primality Testing

Input description: An integer n.

Problem description: Is n a prime number, and if not what are its factors?

Discussion: The dual problems of integer factorization and primality testing have surprisingly many applications for a problem long suspected of being only of mathematical interest. The security of the RSA public-key cryptography system (see Section 18.6 (page 641)) is based on the computational intractability of factoring large integers. As a more modest application, hash table performance typically improves when the table size is a prime number. To get this benefit, an initialization routine must identify a prime near the desired table size. Finally, prime numbers are just interesting to play with. It is no coincidence that programs to generate large primes often reside in the games directory of UNIX systems.

Factoring and primality testing are clearly related problems, although they are quite different algorithmically. There exist algorithms that can demonstrate that an integer is *composite* (i.e. , not prime) without actually giving the factors. To convince yourself of the plausibility of this, note that you can demonstrate the compositeness of any nontrivial integer whose last digit is 0, 2, 4, 5, 6, or 8 without doing the actual division.

The simplest algorithm for both of these problems is brute-force trial division. To factor n, compute the remainder of n/i for all $1 < i \leq \sqrt{n}$. The prime factorization of n will contain at least one instance of every i such that $n/i = \lfloor n/i \rfloor$, unless n is prime. Make sure you handle the multiplicities correctly, and account for any primes larger than $\sqrt{n}$.

Such algorithms can be sped up by using a precomputed table of small primes to avoid testing all possible i. Surprisingly large numbers of primes can be represented in surprisingly little space by using bit vectors (see Section 12.5 (page 385)). A bit vector of all odd numbers less than 1,000,000 fits in under 64 kilobytes. Even tighter encodings become possible by eliminating all multiples of 3 and other small primes.

Although trial division runs in $O(\sqrt{n})$ time, it is *not* a polynomial-time algorithm. The reason is that it only takes $\lg_2 n$ bits to represent n, so trial division takes time exponential in the input size. Considerably faster (but still exponential time) factoring algorithms exist, whose correctness depends upon more substantial number theory. The fastest known algorithm, the *number field sieve*, uses randomness to construct a system of congruences—the solution of which usually gives a factor of the integer. Integers with as many as 200 digits (663 bits) have been factored using this method, although such feats require enormous amounts of computation.

Randomized algorithms make it much easier to test whether an integer is prime. Fermat's little theorem states that $a^{n-1} = 1 (\text{mod } n)$ for all a not divisible by n, provided n is prime. Suppose we pick a random value $1 \leq a < n$ and compute the residue of $a^{n-1} (\text{mod } n)$. If this residue is not 1, we have just proven that n cannot be prime. Such randomized primality tests are very efficient. PGP (see Section 18.6 (page 641)) finds 300+ digit primes using hundreds of these tests in minutes, for use as cryptographic keys.

Although the primes are scattered in a seemingly random way throughout the integers, there is some regularity to their distribution. The *prime number theorem* states that the number of primes less than n (commonly denoted by $\pi(n)$) is approximately $n/\ln n$. Further, there never are large gaps between primes, so in general, one would expect to examine about $\ln n$ integers if one wanted to find the first prime larger than n. This distribution and the fast randomized primality test explain how PGP can find such large primes so quickly.

Implementations: Several general systems for computational number theory are available. PARI is capable of handling complex number-theoretic problems on arbitrary-precision integers (to be precise, limited to 80,807,123 digits on 32-bit machines), as well as reals, rationals, complex numbers, polynomials, and matrices. It is written mainly in C, with assembly code for inner loops on major architectures, and includes more than 200 special predefined mathematical functions. PARI can be used as a library, but it also possesses a calculator mode that gives instant access to all the types and functions. PARI is available at *http://pari.math.u-bordeaux.fr/*

LiDIA (*http://www.cdc.informatik.tu-darmstadt.de/TI/LiDIA/*) is the acronym for the C++ *Library for Computational Number Theory*. It implements several of the modern integer factorization methods.

A Library for doing Number Theory (NTL) is a high-performance, portable C++ library providing data structures and algorithms for manipulating signed, arbitrary length integers, and for vectors, matrices, and polynomials over the integers and over finite fields. It is available at *http://www.shoup.net/ntl/*.

Finally, MIRACL (Multiprecision Integer and Rational Arithmetic C/C++ Library) implements six different integer factorization algorithms, including the quadratic sieve. It is available at *http://www.shamus.ie/*.

Notes: Expositions on modern algorithms for factoring and primality testing include Crandall and Pomerance [CP05] and Yan [Yan03]. More general surveys of computational number theory include Bach and Shallit [BS96] and Shoup [Sho05].

In 2002, Agrawal, Kayal, and Saxena [AKS04] solved a long-standing open problem by giving the first polynomial-time deterministic algorithm to test whether an integer is composite. Their algorithm, which is surprisingly elementary for such an important result, involves a careful analysis of techniques from earlier randomized algorithms. Its existence serves as somewhat of a rebuke to researchers (like me) who shy away from classical open problems due to fear. Dietzfelbinger [Die04] provides a self-contained treatment of this result.

The Miller-Rabin [Mil76, Rab80] randomized primality testing algorithm eliminates problems with Carmichael numbers, which are composite integers that always satisfy Fermat's theorem. The best algorithms for integer factorization include the quadratic-sieve [Pom84] and the elliptic-curve methods [Len87b].

Mechanical sieving devices provided the fastest way to factor integers surprisingly far into the computing era. See [SWM95] for a fascinating account of one such device, built during World War I. Hand-cranked, it proved the primality of $2^{31} - 1$ in 15 minutes of sieving time.

An important problem in computational complexity theory is whether P = NP $\cap$ co-NP. The decision problem "is n a composite number?" used to be the best candidate for a counterexample. By exhibiting the factors of n, it is trivially in NP. It can be shown to be in co-NP, since every prime has a short proof of its primality [Pra75]. The recent proof that composite numbers testing is in P shot down this line of reasoning. For more information on complexity classes, see [GJ79, Joh90].

The integer RSA-129 was factored in eight months using over 1,600 computers. This was particularly noteworthy because in the original RSA paper [RSA78] they had originally predicted such a factorization would take 40 quadrillion years using 1970s technology. Bahr, Boehm, Franke, and Kleinjung hold the current integer factorization record, with their successful attack on the 200-digit integer RSA-200 in May 2005. This required the equivalent of 55 years of computations on a single 2.2 GHz Opteron CPU.

Related Problems: Cryptography (see page 641), high precision arithmetic (see page 423).

INPUT	OUTPUT
$\frac{49578291287491495151508905425869578}{74367436931237242727263358138804367}$	$\frac{2}{3}$

13.9 Arbitrary-Precision Arithmetic

Input description: Two very large integers, x and y.

Problem description: What is $x + y$, $x - y$, $x \times y$, and x/y?

Discussion: Any programming language rising above basic assembler supports single- and perhaps double-precision integer/real addition, subtraction, multiplication, and division. But what if we wanted to represent the national debt of the United States in pennies? One trillion dollars worth of pennies requires 15 decimal digits, which is far more than can fit into a 32-bit integer.

Other applications require *much* larger integers. The RSA algorithm for public-key cryptography recommends integer keys of at least 1000 digits to achieve adequate security. Experimenting with number-theoretic conjectures for fun or research requires playing with large numbers. I once solved a minor open problem [GKP89] by performing an exact computation on the integer $\binom{5906}{2953} \approx 9.93285 \times 10^{1775}$.

What should you do when you need large integers?

- *Am I solving a problem instance requiring large integers, or do I have an embedded application?* – If you just need the answer to a specific problem with large integers, such as in the number theory application above, you should consider using a computer algebra system like Maple or Mathematica. These provide arbitrary-precision arithmetic as a default and use nice Lisp-like programming languages as a front end—together often reducing your problem to a 5- to 10- line program.

  If you have an embedded application requiring high-precision arithmetic instead, you should use an existing arbitrary precision math library. You are likely to get additional functions beyond the four basic operations for computing things like greatest common divisor in the bargain. See the Implementations section for details.

- *Do I need high- or arbitrary-precision arithmetic?* – Is there an upper bound on how big your integers can get, or do you really need *arbitrary*-precision—i.e. , unbounded. This determines whether you can use a fixed-length array to represent your integers as opposed to a linked-list of digits. The array is likely to be simpler and will not prove a constraint in most applications.

- *What base should I do arithmetic in?* – It is perhaps simplest to implement your own high-precision arithmetic package in decimal, and thus represent each integer as a string of base-10 digits. However, it is far more efficient to use a higher base, ideally equal to the square root of the largest integer supported fully by hardware arithmetic.

  Why? The higher the base, the fewer digits we need to represent a number. Compare 64 decimal with 1000000 binary. Since hardware addition usually takes one clock cycle independent of value of the actual numbers, best performance is achieved using the highest supported base. The factor limiting us to base $b = \sqrt{maxint}$ is the desire to avoid overflow when multiplying two of these "digits" together.

  The primary complication of using a larger base is that integers must be converted to and from base-10 for input and output. The conversion is easily performed once all four high-precision arithmetical operations are supported.

- *How low-level are you willing to get for fast computation?* – Hardware addition is much faster than a subroutine call, so you take a significant hit on speed using high-precision arithmetic when low-precision arithmetic suffices. High-precision arithmetic is one of few problems in this book where inner loops in assembly language prove the right idea to speed things up. Similarly, using bit-level masking and shift operations instead of arithmetical operations can be a win if you really understand the machine integer representation.

The algorithm of choice for each of the five basic arithmetic operations is as follows:

- *Addition* – The basic schoolhouse method of lining up the decimal points and then adding the digits from right to left with "carries" runs to time linear in the number of digits. More sophisticated carry-look-ahead parallel algorithms are available for low-level hardware implementation. They are presumably used on your microprocessor for low-precision addition.

- *Subtraction* – By fooling with the sign bits of the numbers, subtraction can be a special considered case of addition: $(A - (-B)) = (A + B)$. The tricky part of subtraction is performing the "borrow." This can be simplified by always subtracting from the number with the larger absolute value and adjusting the signs afterwards, so we can be certain there will always be something to borrow from.

- *Multiplication* – Repeated addition will take exponential time on large integers, so stay away from it. The digit-by-digit schoolhouse method is reasonable to program and will work much better, presumably well enough for your application. On very large integers, Karatsuba's $O(n^{1.59})$ divide-and-conquer algorithm wins. Dan Grayson, author of Mathematica's arbitrary-precision arithmetic, found that the switch-over happened at well under 100 digits.

Even faster for very large integers is an algorithm based on Fourier transforms. Such algorithms are discussed in Section 13.11 (page 431).

- *Division* – Repeated subtraction will take exponential time, so the easiest reasonable algorithm to use is the long-division method you hated in school. This is fairly complicated, requiring arbitrary-precision multiplication and subtraction as subroutines, as well as trial-and-error, to determine the correct digit at each position of the quotient.

  In fact, integer division can be reduced to integer multiplication, although in a nontrivial way, so if you are implementing asymptotically fast multiplication, you can reuse that effort in long division. See the references below for details.

- *Exponentiation* – We can compute a^n using $n-1$ multiplications, by computing $a \times a \times \ldots \times a$. However, a much better divide-and-conquer algorithm is based on the observation that $n = \lfloor n/2 \rfloor + \lceil n/2 \rceil$. If n is even, then $a^n = (a^{n/2})^2$. If n is odd, then $a^n = a(a^{\lfloor n/2 \rfloor})^2$. In either case, we have halved the size of our exponent at the cost of at most two multiplications, so $O(\lg n)$ multiplications suffice to compute the final value:

```
function power(a, n)
    if (n = 0) return(1)
    x = power(a, ⌊n/2⌋)
    if (n is even) then return(x^2)
        else return(a × x^2)
```

High- but not arbitrary-precision arithmetic can be conveniently performed using the Chinese remainder theorem and modular arithmetic. The *Chinese remainder theorem* states that an integer between 1 and $P = \prod_{i=1}^{k} p_i$ is uniquely determined by its set of residues mod p_i, where each p_i, p_j are relatively prime integers. Addition, subtraction, and multiplication (but not division) can be supported using such residue systems, with the advantage that large integers can be manipulated without complicated data structures.

Many of these algorithms for computations on long integers can be directly applied to computations on polynomials. See the references for more details. A particularly useful algorithm is Horner's rule for fast polynomial evaluation. When $P(x) = \sum_{i=0}^{n} c_i \cdot x^i$ is blindly evaluated term by term, $O(n^2)$ multiplications will be performed. Much better is observing that $P(x) = c_0 + x(c_1 + x(c_2 + x(c_3 + \ldots)))$, the evaluation of which uses only a linear number of operations.

Implementations: All major commercial computer algebra systems incorporate high-precision arithmetic, including Maple, Mathematica, Axiom, and Macsyma. If you have access to one of these, this is your best option for a quick, nonembedded

application. The rest of this section focuses on source code available for embedded applications.

The premier C/C++ library for fast, arbitrary-precision is the GNU Multiple Precision Arithmetic Library (GMP), which operates on signed integers, rational numbers, and floating point numbers. It is widely used and well-supported, and available at *http://gmplib.org/*.

The `java.math BigInteger` class provides arbitrary-precision analogues to all of Java's primitive integer operators. `BigInteger` provides additional operations for modular arithmetic, GCD calculation, primality testing, prime generation, bit manipulation, and a few other miscellaneous operations.

A lower-performance, less-tested, but more personal implementation of high-precision arithmetic appears in the library from my book *Programming Challenges* [SR03]. See Section 19.1.10 (page 661) for details.

Several general systems for computational number theory are available. Each of these supports operations of arbitrary-precision integers. Information about the PARI, LiDIA, NTL and MIRACL number-theoretic libraries can be found in Section 13.8 (page 420).

ARPREC is a C++/Fortran-90 arbitrary precision package with an associated interactive calculator. MPFUN90 is a similar package written exclusively in Fortran-90. Both are available at *http://crd.lbl.gov/~dhbailey/mpdist/*. Algorithm 693 [Smi91] of the *Collected Algorithms of the ACM* is a Fortran implementation of floating-point, multiple-precision arithmetic. See Section 19.1.5 (page 659).

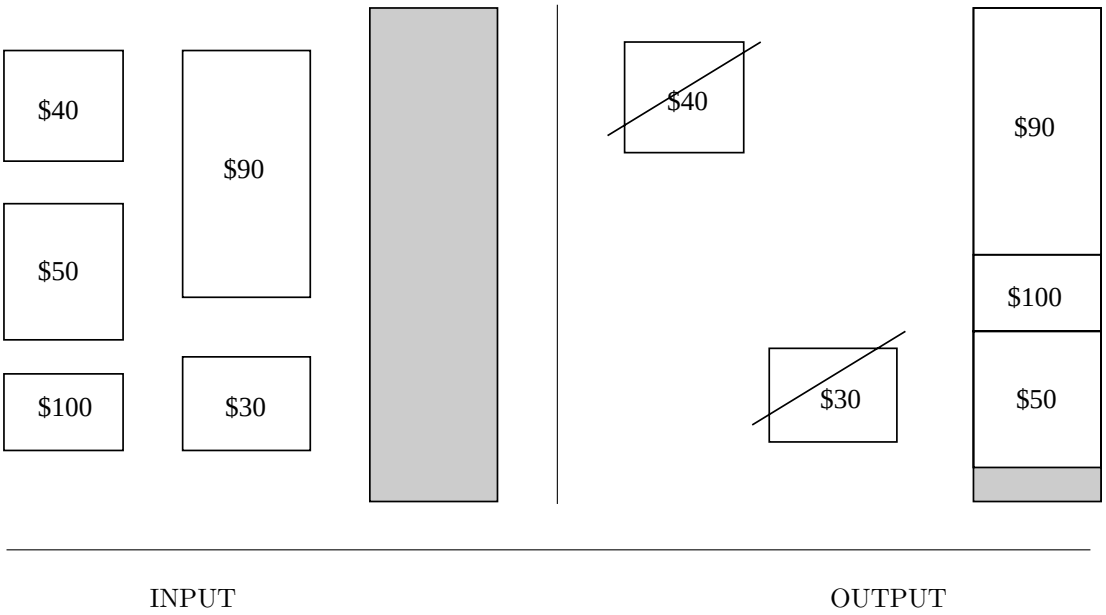
Notes: Knuth [Knu97b] is the primary reference on algorithms for all basic arithmetic operations, including implementations of them in the MIX assembly language. Bach and Shallit [BS96] and Shoup [Sho05] provide more recent treatments of computational number theory.

Expositions on the $O(n^{1.59})$-time divide-and-conquer algorithm for multiplication [KO63] include [AHU74, Man89]. An FFT-based algorithm multiplies two n-bit numbers in $O(n \lg n \lg \lg n)$ time and is due to Schönhage and Strassen [SS71]. Expositions include [AHU74, Knu97b]. The reduction between integer division and multiplication is presented in [AHU74, Knu97b]. Applications of fast multiplication to other arithmetic operations are presented by Bernstein [Ber04b]

Good expositions of algorithms for modular arithmetic and the Chinese remainder theorem include [AHU74, CLRS01]. A good exposition of circuit-level algorithms for elementary arithmetic algorithms is [CLRS01].

Euclid's algorithm for computing the greatest common divisor of two numbers is perhaps the oldest interesting algorithm. Expositions include [CLRS01, Man89].

Related Problems: Factoring integers (see page 420), cryptography (see page 641).



13.10 Knapsack Problem

Input description: A set of items $S = \{1, \ldots, n\}$, where item i has size s_i and value v_i. A knapsack capacity is C.

Problem description: Find the subset $S' \subset S$ that maximizes the value of $\sum_{i \in S'} v_i$, given that $\sum_{i \in S'} s_i \leq C$; i.e. , all the items fit in a knapsack of size C.

Discussion: The knapsack problem arises in resource allocation with financial constraints. How do you select what things to buy given a fixed budget? Everything has a cost and value, so we seek the most value for a given cost. The name *knapsack problem* invokes the image of the backpacker who is constrained by a fixed-size knapsack, and so must fill it only with the most useful and portable items.

The most common formulation is the *0/1 knapsack problem*, where each item must be put entirely in the knapsack or not included at all. Objects cannot be broken up arbitrarily, so it is not fair taking one can of Coke from a six-pack or opening a can to take just a sip. It is this 0/1 property that makes the knapsack problem hard, for a simple greedy algorithm finds the optimal selection when we are allowed to subdivide objects. We compute the "price per pound" for each item, and take the most expensive item or the biggest part thereof until the knapsack is full. Repeat with the next most expensive item. Unfortunately, the 0/1 constraint is usually inherent in most applications.

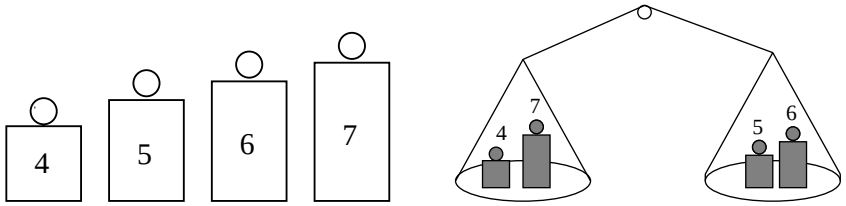


Figure 13.1: Integer partition is a special case of the knapsack problem

Issues that arise in selecting the best algorithm include:

- *Does every item have the same cost/value or the same size?* – When all items are worth exactly the same amount, we maximize our value by taking the greatest number of items. Therefore, the optimal solution is to sort the items in order of increasing size and insert them into the knapsack in this order until no more fit. The problem is similarly solved when each object has the same size but the costs are different. Sort by cost, and take the cheapest elements first. These are the easy cases of knapsack.

- *Does each item have the same "price per pound"?* – In this case, our problem is equivalent to ignoring the price and just trying to minimize the amount of empty space left in the knapsack. Unfortunately, even this restricted version is NP-complete, so we cannot expect an efficient algorithm that always solves the problem. Don't lose hope, however, because knapsack proves to be an "easy" hard problem, and one that can usually be handled with the algorithms described below.

  An important special case of a constant "price-per-pound" knapsack is the *integer partition* problem, presented in cartoon form in Figure 13.1. Here, we seek to partition the elements of S into two sets A and B such that $\sum_{a \in A} a = \sum_{b \in B}$, or alternately make the difference as small as possible. Integer partition can be thought of as bin packing into two equal-sized bins or knapsack with a capacity of half the total weight, so all three problems are closely related and NP-complete.

  The constant "price-per-pound" knapsack problem is often called the *subset sum* problem, because we seek a subset of items that adds up to a specific target number C; i.e. , the capacity of our knapsack.

- *Are all the sizes relatively small integers?* – When the sizes of the items and the knapsack capacity C are all integers, there exists an efficient dynamic programming algorithm to find the optimal solution in time $O(nC)$ and $O(C)$ space. Whether this works for you depends upon how big C is. It is great for $C \leq 1{,}000$, but not so great for $C \geq 10{,}000{,}000$.

The algorithm works as follows: Let S' be a set of items, and let $C[i, S']$ be true if and only if there is a subset of S' whose size adds up exactly to i. Thus, $C[i, \emptyset]$ is false for all $1 \leq i \leq C$. One by one we add a new item s_j to S' and update the affected values of $C[i, S']$. Observe that $C[i, S' \cup s_j] =$ true iff $C[i, S']$ or $C[i - s_j, S']$ is true, since we either use s_j in realizing the sum or we don't. We identify all sums that can be realized by performing n sweeps through all C elements—one for each s_j, $1 \leq j \leq n$—and so updating the array. The knapsack solution is given by the largest index of a true element of the largest realizable size. To reconstruct the winning subset, we must also store the name of the item number that turned $C[i]$ from false to true for each $1 \leq i \leq C$ and then scan backwards through the array.

This dynamic programming formulation ignores the values of the items. To generalize the algorithm, use each element of the array to store the value of the best subset to date summing up to i. We now update when the sum of the cost of $C[i - s_j, S']$ plus the cost of s_j is better than the previous cost of $C[i]$.

- *What if I have multiple knapsacks?* – When there are multiple knapsacks, your problem might be better thought of as a bin-packing problem. Check out Section 17.9 (page 595) for bin-packing/cutting-stock algorithms. That said, algorithms for optimizing over multiple knapsacks are provided in the Implementations section below.

Exact solutions for large capacity knapsacks can be found using integer programming or backtracking. A 0/1 integer variable x_i is used to denote whether item i is present in the optimal subset. We maximize $\sum_{i=1}^{n} x_i \cdot v_i$ given the constraint that $\sum_{i=1}^{n} x_i \cdot s_i \leq C$. Integer programming codes are discussed in Section 13.6 (page 411).

Heuristics must be used when exact solutions prove too costly to compute. The simple greedy heuristic inserts items according to the maximum "price per pound" rule described previously. Often this heuristic solution is close to optimal, but it can be arbitrarily bad depending upon the problem instance. The "price per pound" rule can also be used to reduce the problem size in exhaustive search-based algorithms by eliminating "cheap but heavy" objects from future consideration.

Another heuristic is based on *scaling*. Dynamic programming works well if the knapsack capacity is a reasonably small integer, say $\leq C_s$. But what if we have a problem with capacity $C > C_s$? We scale down the sizes of all items by a factor of C/C_s, round the size down to the nearest integer, and then use dynamic programming on the scaled items. Scaling works well in practice, especially when the range of sizes of items is not too large.

Implementations: Martello and Toth's collection of Fortran implementations of algorithms for a variety of knapsack problem variants are available at *http://www.or.deis.unibo.it/kp.html*. An electronic copy of the associated book [MT90a] has also been generously made available.

David Pisinger maintains a well-organized collection of C-language codes for knapsack problems and related variants like bin packing and container loading. These are available at *http://www.diku.dk/∼pisinger/codes.html*. The strongest code is based on the dynamic programming algorithm of [MPT99].

Algorithm 632 [MT85] of the *Collected Algorithms of the ACM* is a Fortran code for the 0/1 knapsack problem, with the twist that it supports multiple knapsacks. See Section 19.1.5 (page 659).

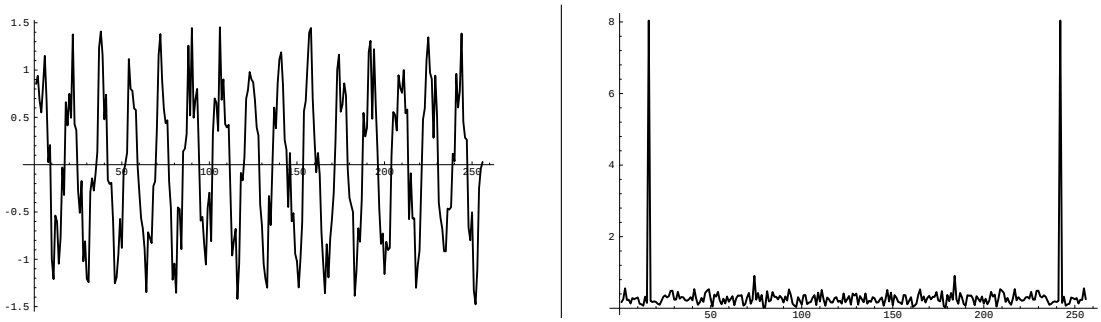
Notes: Keller, Pferschy, and Pisinger [KPP04] is the most current reference on the knapsack problem and variants. Martello and Toth's book [MT90a] and survey article [MT87] are standard references on the knapsack problem, including both theoretical and experimental results. An excellent exposition on integer programming approaches to knapsack problems appears in [SDK83]. See [MPT00] for a computational study of algorithms for 0-1 knapsack problems.

A polynomial-time approximation scheme is an algorithm that approximates the optimal solution of a problem in time polynomial in both its size and the approximation factor ϵ.

This very strong condition implies a smooth tradeoff between running time and approximation quality. Good expositions on polynomial-time approximation schemes [IK75] for knapsack and subset sum includes [BvG99, CLRS01, GJ79, Man89].

The first algorithm for generalized public key encryption by Merkle and Hellman [MH78] was based on the hardness of the knapsack problem. See [Sch96] for an exposition.

Related Problems: Bin packing (see page 595), integer programming (see page 411).



INPUT OUTPUT

13.11 Discrete Fourier Transform

Input description: A sequence of n real or complex values h_i, $0 \leq i \leq n-1$, sampled at uniform intervals from a function h.

Problem description: The discrete Fourier transform $H_m = \sum_{k=0}^{n-1} h_k e^{2\pi ikm/n}$ for $0 \leq m \leq n-1$.

Discussion: Although computer scientists tend to be fairly ignorant about Fourier transforms, electrical engineers and signal processors eat them for breakfast. Functionally, Fourier transforms provide a way to convert samples of a standard time-series into the *frequency domain*. This provides a dual representation of the function in which certain operations become easier than in the time domain. Applications of Fourier transforms include:

- *Filtering* – Taking the Fourier transform of a function is equivalent to representing it as the sum of sine functions. By eliminating undesirable high- and/or low-frequency components (i.e. , dropping some of the sine functions) and taking an inverse Fourier transform to get us back into the time domain, we can filter an image to remove noise and other artifacts. For example, the sharp spike in the figure above represents the period of the single sine function that closely models the input data. The rest is noise.
- *Image compression* – A smoothed, filtered image contains less information than the original, while retaining a similar appearance. By eliminating the coefficients of sine functions that contribute relatively little to the image, we can reduce the size of the image at little cost in image fidelity.
- *Convolution and deconvolution* – Fourier transforms can efficiently compute convolutions of two sequences. A *convolution* is the pairwise product of elements from two different sequences, such as in multiplying two n-variable

polynomials f and g or comparing two character strings. Implementing such products directly takes $O(n^2)$, while the fast Fourier transform led to a $O(n \lg n)$ algorithm.

Another example comes from image processing. Because a scanner measures the darkness of an image patch instead of a single point, the scanned input is always blurred. A reconstruction of the original signal can be obtained by deconvoluting the input signal with a Gaussian point-spread function.

- *Computing the correlation of functions* – The *correlation function* of two functions $f(t)$ and $g(t)$ is defined by

$$z(t) = \int_{-\infty}^{\infty} f(\tau)g(t+\tau)d\tau$$

and can be easily computed using Fourier transforms. When two functions are similar in shape but one is shifted relative to the other (such as $f(t) = \sin(t)$ and $g(t) = \cos(t)$), the value of $z(t_0)$ will be large at this shift offset t_0. As an application, suppose that we want to detect whether there are any funny periodicities in our random-number generator. We can generate a large series of random numbers, turn them into a time series (the ith number at time i), and take the Fourier transform of this series. Any funny spikes will correspond to potential periodicities.

The discrete Fourier transform takes as input n complex numbers h_k, $0 \leq k \leq n-1$, corresponding to equally spaced points in a time series, and outputs n complex numbers H_k, $0 \leq k \leq n-1$, each describing a sine function of given frequency. The discrete Fourier transform is defined by

$$H_m = \sum_{k=0}^{n-1} h_k e^{-2\pi ikm/n}$$

and the inverse Fourier transform is defined by

$$h_m = \frac{1}{n} \sum_{k=0}^{n-1} H_k e^{2\pi ikm/n}$$

which enables us move easily between h and H.

Since the output of the discrete Fourier transform consists of n numbers, each of which is computed using a formula on n numbers, they can be computed in $O(n^2)$ time. The fast Fourier transform (FFT) is an algorithm that computes the discrete Fourier transform in $O(n \log n)$. This is arguably the most important algorithm known, for it opened the door to modern signal processing. Several different algorithms call themselves FFTs, all of which are based on a divide-and-conquer approach. Essentially, the problem of computing the discrete Fourier transform on

n points is reduced to computing two transforms on $n/2$ points each, and is then applied recursively.

The FFT usually assumes that n is a power of two. If this is not the case, you are usually better off padding your data with zeros to create $n = 2^k$ elements rather than hunting for a more general code.

Many signal-processing systems have strong real-time constraints, so FFTs are often implemented in hardware, or at least in assembly language tuned to the particular machine. Be aware of this possibility if the codes prove too slow.

Implementations: FFTW is a C subroutine library for computing the discrete Fourier transform in one or more dimensions, with arbitrary input size, and supporting both real and complex data. It is the clear choice among freely available FFT codes. Extensive benchmarking proves it to be the "Fastest Fourier Transform in the West." Interfaces to Fortran and C++ are provided. FFTW received the 1999 J. H. Wilkinson Prize for Numerical Software. It is available at *http://www.fftw.org/*.

FFTPACK is a package of Fortran subprograms for the fast Fourier transform of periodic and other symmetric sequences, written by P. Swartzrauber. It includes complex, real, sine, cosine, and quarter-wave transforms. FFTPACK resides on Netlib (see Section 19.1.5 (page 659)) at *http://www.netlib.org/fftpack*. The GNU Scientific Library for C/C++ provides a reimplementation of FFTPACK. See *http://www.gnu.org/software/gsl/*.

Algorithm 545 [Fra79] of the *Collected Algorithms of the ACM* is a Fortran implementation of the fast Fourier transform optimizing virtual memory performance. See Section 19.1.5 (page 659) for further information.

Notes: Bracewell [Bra99] and Brigham [Bri88] are excellent introductions to Fourier transforms and the FFT. See also the exposition in [PFTV07]. Credit for inventing the fast Fourier transform is usually given to Cooley and Tukey [CT65], but see [Bri88] for a complete history.

A cache-oblivious algorithm for the fast Fourier transform is given in [FLPR99]. This paper first introduced the notion of cache-oblivious algorithms. The FFTW is based on this algorithm. See [FJ05] for more on the design of the FFTW.

An interesting divide-and-conquer algorithm for polynomial multiplication [KO63] does the job in $O(n^{1.59})$ time and is discussed in [AHU74, Man89]. An FFT-based algorithm that multiplies two n-bit numbers in $O(n \lg n \lg \lg n)$ time is due to Schönhage and Strassen [SS71] and is presented in [AHU74].

It is an open question of whether complex variables are really fundamental to fast algorithms for convolution. Fortunately, fast convolution can be used as a black box in most applications. Many variants of string matching are based on fast convolution [Ind98].

In recent years, wavelets have been proposed to replace Fourier transforms in filtering. See [Wal99] for an introduction to wavelets.

Related Problems: Data compression (see page 637), high-precision arithmetic (see page 423).

14

Combinatorial Problems

We now consider several algorithmic problems of a purely combinatorial nature. These include sorting and permutation generations, both of which were among the first non-numerical problems arising on electronic computers. Sorting can be viewed as identifying or imposing a total order on the keys, while searching and selection involve identifying specific keys based on their position in this total order.

The rest of this section deals with other combinatorial objects, such as permutations, partitions, subsets, calendars, and schedules. We are particularly interested in algorithms that *rank* and *unrank* combinatorial objects—i.e. , that map each distinct object to and from a unique integer. Rank and unrank operations make many other tasks simple, such as generating random objects (pick a random number and unrank) or listing all objects in order (iterate from 1 to n and unrank).

We conclude with the problem of generating graphs. Graph algorithms are more fully presented in subsequent sections of the catalog.

Books on general combinatorial algorithms, in this restricted sense, include:

- *Nijenhuis and Wilf* [NW78] – This book specializes in algorithms for constructing basic combinatorial objects such as permutations, subsets, and partitions. Such algorithms are often very short but hard to locate and usually are surprisingly subtle. Fortran programs for all of the algorithms are provided, as well as a discussion of the theory behind each of them. See Section 19.1.10 for details.

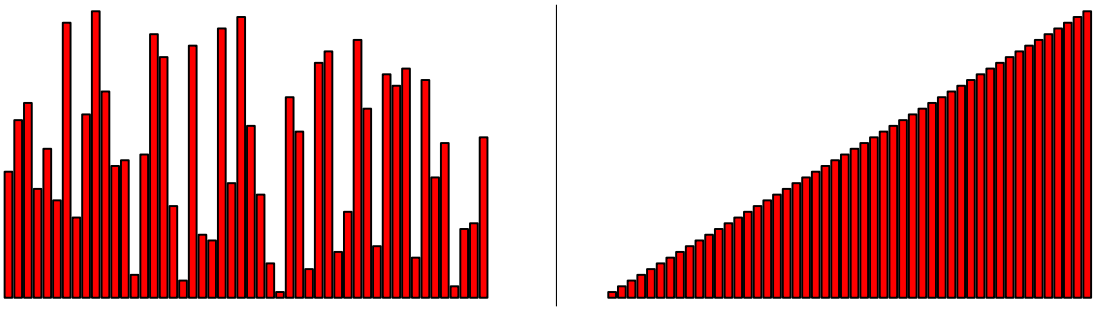
- *Kreher and Stinson* [KS99] – The most recent book on combinatorial generation algorithms, with additional particular focus on algebraic problems such as isomorphism and dealing with symmetry.

S.S. Skiena, *The Algorithm Design Manual*, 2nd ed., DOI: 10.1007/978-1-84800-070-4_14,
© Springer-Verlag London Limited 2008

- *Knuth* [Knu97a, Knu98] – The standard reference on searching and sorting, with significant material on combinatorial objects such as permutations. New material on the generation of permutations [Knu05a], subsets and partitions [Knu05b], and trees [Knu06] has been released on "fasciles,"—short paperback chunks of what is slated to be the mythical Volume 4.

- *Stanton and White* [SW86a] – An undergraduate combinatorics text with algorithms for generating permutations, subsets, and set partitions. It contains relevant programs in Pascal.

- *Pemmaraju and Skiena* [PS03] – This description of *Combinatorica*, a library of over 400 Mathematica functions for generating combinatorial objects and graph theory (see Section 19.1.9), provides a distinctive view of how different algorithms can fit together. Its second author is considered qualified to write a manual on algorithm design.



INPUT OUTPUT

14.1 Sorting

Input description: A set of n items.

Problem description: Arrange the items in increasing (or decreasing) order.

Discussion: Sorting is the most fundamental algorithmic problem in computer science. Learning the different sorting algorithms is like learning scales for a musician. Sorting is the first step in solving a host of other algorithm problems, as shown in Section 4.2 (page 107). Indeed, *"when in doubt, sort"* is one of the first rules of algorithm design.

Sorting also illustrates all the standard paradigms of algorithm design. The result is that most programmers are familiar with many different sorting algorithms, which sows confusion as to which should be used for a given application. The following criteria can help you decide:

- *How many keys will you be sorting?* – For small amounts of data (say $n \leq 100$), it really doesn't matter much which of the quadratic-time algorithms you use. Insertion sort is faster, simpler, and less likely to be buggy than bubblesort. Shellsort is closely related to, but much faster than, insertion sort, but it involves looking up the right insert sequences in Knuth [Knu98].

  When you have more than 100 items to sort, it is important to use an $O(n \lg n)$-time algorithm like heapsort, quicksort, or mergesort. There are various partisans who favor one of these algorithms over the others, but since it can be hard to tell which is fastest, it usually doesn't matter.

  Once you get past (say) 5,000,000 items, it is important to start thinking about external-memory sorting algorithms that minimize disk access. Both types of algorithm are discussed below.

- *Will there be duplicate keys in the data?* – The sorted order is completely defined if all items have distinct keys. However, when two items share the same key, something else must determine which one comes first. In many applications it doesn't matter, so any sorting algorithm suffices. Ties are often broken by sorting on a secondary key, like the first name or initial when the family names collide.

  Occasionally, ties need to be broken by their initial position in the data set. Suppose the 5th and 27th items of the initial data set share the same key. This means the 5th item must appear before the 27th in the final order. A *stable* sorting algorithm preserves the original ordering in case of ties. Most of the quadratic-time sorting algorithms are stable, while many of the $O(n \lg n)$ algorithms are not. If it is important that your sort be stable, it is probably better to explicitly use the initial position as a secondary key in your comparison function rather than trust the stability of your implementation.

- *What do you know about your data?* – You can often exploit special knowledge about your data to get it sorted faster or more easily. Of course, general sorting is a fast $O(n \lg n)$ operation, so if the time spent sorting is really the bottleneck in your application, you are a fortunate person indeed.

  - *Has the data already been partially sorted?* If so, certain algorithms like insertion sort perform better than they otherwise would.
  - *Do you know the distribution of the keys?* If the keys are randomly or uniformly distributed, a *bucket* or *distribution sort* makes sense. Throw the keys into bins based on their first letter, and recur until each bin is small enough to sort by brute force. This is very efficient when the keys get evenly distributed into buckets. However, bucket sort would perform very badly sorting names on the membership roster of the "Smith Society."
  - *Are your keys very long or hard to compare?* If your keys are long text strings, it might pay to use a relatively short prefix (say ten characters) of each key for an initial sort, and then resolve ties using the full key. This is particularly important in external sorting (see below), since you don't want to waste your fast memory on the dead weight of irrelevant detail.

    Another idea might be to use radix sort. This always takes time linear in the number of characters in the file, instead of $O(n \lg n)$ times the cost of comparing two keys.
  - *Is the range of possible keys very small?* If you want to sort a subset of, say, $n/2$ distinct integers, each with a value from 1 to n, the fastest algorithm would be to initialize an n-element bit vector, turn on the bits corresponding to keys, then scan from left to right and report the positions with true bits.

- *Do I have to worry about disk accesses?* – In massive sorting problems, it may not be possible to keep all data in memory simultaneously. Such a problem is called *external sorting*, because one must use an external storage device. Traditionally, this meant tape drives, and Knuth [Knu98] describes a variety of intricate algorithms for efficiently merging data from different tapes. Today, it usually means virtual memory and swapping. Any sorting algorithm will run using virtual memory, but most will spend all their time swapping.

  The simplest approach to external sorting loads the data into a B-tree (see Section 12.1 (page 367)) and then does an in-order traversal of the tree to read the keys off in sorted order. Real high-performance sorting algorithms are based on multiway-mergesort. Files containing portions of the data are sorted into runs using a fast internal sort, and then files with these sorted runs are merged in stages using 2- or k-way merging. Complicated merging patterns and buffer management based on the properties of the external storage device can be used to optimize performance.

- *How much time do you have to write and debug your routine?* – If I had under an hour to deliver a working routine, I would probably just implement a simple selection sort. If I had an afternoon to build an efficient sort routine, I would probably use heapsort, for it delivers reliable performance without tuning.

The best general-purpose internal sorting algorithm is quicksort (see Section 4.2 (page 107)), although it requires tuning effort to achieve maximum performance. Indeed, you are much better off using a library function instead of coding it yourself. A poorly written quicksort will likely run more slowly than a poorly written heapsort.

If you are determined to implement your own quicksort, use the following heuristics, which make a big difference in practice:

- *Use randomization* – By randomly permuting (see Section 14.4 (page 448)) the keys before sorting, you can eliminate the potential embarrassment of quadratic-time behavior on nearly-sorted data.

- *Median of three* – For your pivot element, use the median of the first, last, and middle elements of the array to increase the likelihood of partitioning the array into roughly equal pieces. Some experiments suggest using a larger sample on big subarrays and a smaller sample on small ones.

- *Leave small subarrays for insertion sort* – Terminating the quicksort recursion and switching to insertion sort makes sense when the subarrays get small, say fewer than 20 elements. You should experiment to determine the best switchpoint for your implementation.

- *Do the smaller partition first* – Assuming that your compiler is smart enough to remove tail recursion, you can minimize run-time memory by processing

the smaller partition before the larger one. Since successive stored calls are at most half as large as the previous one, only $O(\lg n)$ stack space is needed.

Before you get started, see Bentley's article on building a faster quicksort [Ben92b].

Implementations: The best freely available sort program is presumably GNU sort, part of the GNU core utilities library. See *http://www.gnu.org/software/coreutils/*. Be aware that there are also commercial vendors of high-performance external sorting programs. These include Cosort (*www.cosort.com*), Syncsort (*www.syncsort.com*) and Ordinal Technology (*www.ordinal.com*).

Modern programming languages provide libraries offering complete and efficient container implementations. Thus, you should never need to implement your own sort routine. The C standard library contains `qsort`, a generic implementation of (presumably) quicksort. The C++ *Standard Template Library* (STL) provides both `sort` and `stable_sort` methods. It is available with documentation at *http://www.sgi.com/tech/stl/*. See Josuttis [Jos99], Meyers [Mey01] and Musser [MDS01] for more detailed guides to using STL and the C++ standard library.

Java Collections (JC), a small library of data structures, is included in the `java.util` package of Java standard edition (*http://java.sun.com/javase/*). In particular, `SortedMap` and `SortedSet` classes are provided.

For a C++ implementation of an cache-oblivious algorithm (*funnelsort*), check out *http://kristoffer.vinther.name/projects/funnelsort/*. Benchmarks attest to its excellent performance.

There are a variety of websites that provide applets/animations of all the basic sorting algorithms, including bubblesort, heapsort, mergesort, quicksort, radix sort, and shellsort. Many of these are quite interesting to watch. Indeed, sorting is the canonical problem for algorithm animation. Representative examples include Harrison (*http://www.cs.ubc.ca/spider/harrison/Java/sorting-demo.html*) and Bentley [Ben99] (*http://www.cs.bell-labs.com/cm/cs/pearls/sortanim.html*).

Notes: Knuth [Knu98] is the best book that has been written on sorting and indeed is the best book that will ever be written on sorting. It is now over thirty years old, but remains fascinating reading. One area that has developed since Knuth is sorting under presortedness measures, surveyed in [ECW92]. A noteworthy reference on sorting is [GBY91], which includes pointers to algorithms for partially sorted data and includes implementations in C and Pascal for all of the fundamental algorithms.

Expositions on the basic internal sorting algorithms appear in every algorithms text. Heapsort was first invented by Williams [Wil64]. Quicksort was invented by Hoare [Hoa62], with careful analysis and implementation by Sedgewick [Sed78]. Von Neumann is credited with having produced the first implementation of mergesort on the EDVAC in 1945. See Knuth for a full discussion of the history of sorting, dating back to the days of punch-card tabulating machines.

The primary competitive forum for high-performance sorting is an annual competition initiated by the late Jim Gray. See *http://research.microsoft.com/barc/SortBenchmark/* for current and previous results, which are are either inspiring or depressing depending

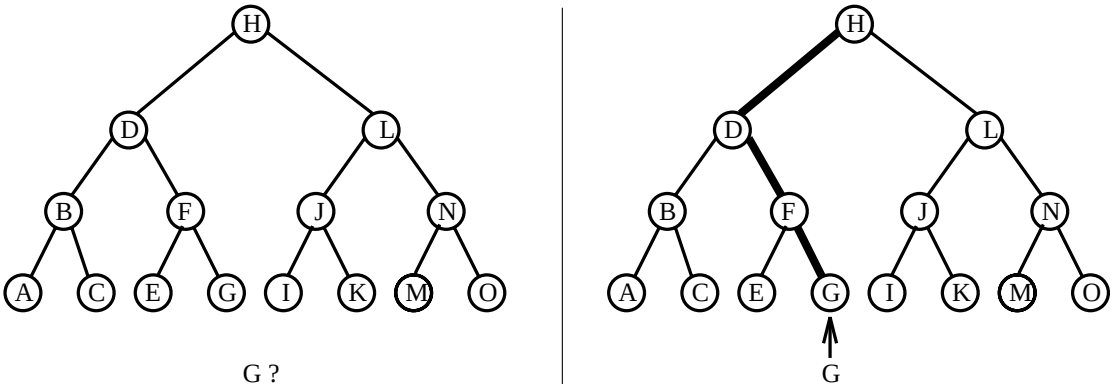
upon how you look at it. The magnitude of progress is inspiring (the million-record instances of the original benchmarks are now too small to bother with) but it is depressing (to me) the extent that systems/memory management issues thoroughly trump the combinatorial/algorithmic aspects of sorting.

Modern attempts to engineer high-performance sort programs include work on both cache-conscious [LL99] and cache-oblivious [BFV07] sorting.

Sorting has a well-known $\Omega(n \lg n)$ lower bound under the algebraic decision tree model [BO83]. Determining the exact number of comparisons required for sorting n elements, for small values of n, has generated considerable study. See [Aig88, Raw92] for expositions and Peczarski [Pec04, Pec07] for the latest results.

This lower-bound does not hold under different models of computation. Fredman and Willard [FW93] present an $O(n\sqrt{\lg n})$ algorithm for sorting under a model of computation that permits arithmetic operations on keys. See Andersson [And05] for a survey of algorithms for fast sorting on such nonstandard models of computation.

Related Problems: Dictionaries (see page 367), searching (see page 441), topological sorting (see page 481).



INPUT OUTPUT

14.2 Searching

Input description: A set of n keys S, and a query key q.

Problem description: Where is q in S?

Discussion: "Searching" is a word that means different things to different people. Searching for the global maximum or minimum of a function is the problem of *unconstrained optimization* and is discussed in Section 13.5 (page 407). Chess-playing programs select the best move to make via an exhaustive search of possible moves using a variation of backtracking (see Section 7.1 (page 231)).

Here we consider the task of searching for a key in a list, array, or tree. Dictionary data structures maintain efficient access to sets of keys under insertion and deletion and are discussed in Section 12.1 (page 367). Typical dictionaries include binary trees and hash tables.

We treat searching as a problem distinct from dictionaries because simpler and more efficient solutions emerge when our primary interest is static searching without insertion/deletion. These little data structures can yield large performance improvements when properly employed in an innermost loop. Also, ideas such as binary search and self-organization apply to other problems and well justify our attention.

Our two basic approaches are sequential search and binary search. Both are simple, yet have interesting and subtle variations. In *sequential search*, we start from the front of our list/array of keys and compare each successive item against the key until we find a match or reach the end. In *binary search*, we start with a sorted array of keys. To search for key q, we compare q to the middle key $S_{n/2}$. If q is before $S_{n/2}$, it must reside in the top half of our set; if not, it must reside in the

bottom half of our set. By repeating this process on the correct half, we find the key using $\lceil \lg n \rceil$ comparisons. This is a big win over the $n/2$ comparisons we expect with sequential search. See Section 4.9 (page 132) for more on binary search.

A sequential search is the simplest algorithm, and likely to be fastest on up to about 20 elements. Beyond (say) 100 elements, binary search will clearly be more efficient than sequential search, easily justifying the cost of sorting if there will be multiple queries. Other issues come into play, however, in identifying the proper variant of the algorithm:

- *How much time can you spend programming?* – A binary search is a notoriously tricky algorithm to program correctly. It took seventeen years after its invention until the first *correct* version of a binary search was published! Don't be afraid to start from one of the implementations described below. Test it completely by writing a driver that searches for every key in the set S as well as between the keys.

- *Are certain items accessed more often than other ones?* – Certain English words (such as "the") are much more likely to occur than others (such as "defenestrate"). We can reduce the number of comparisons in a sequential search by putting the most popular words on the top of the list and the least popular ones at the bottom. Nonuniform access is usually the rule, not the exception. Many real-world distributions are governed by *power laws*. A classic example is word use in English, which is fairly accurately modeled by *Zipf's law*. Under *Zipf's law*, the ith most frequently accessed key is selected with probability $(i-1)/i$ times the probability of the $(i-1)$st most popular key, for all $1 \leq i \leq n$.

  Knowledge of access frequencies is easy to exploit with sequential search. But the issue is more complicated with binary trees. We want popular keys close to the root (so we hit them quickly) but not at the expense of losing balance and degenerating into sequential search. The answer is to employ a dynamic programming algorithm to find the *optimal binary search tree*. The key observation is that each possible root node i partitions the space of keys into those to the left of i and those to the right; each of which should be represented by an optimal binary search tree on a smaller subrange of keys. The root of the optimal tree is selected to minimize the expected search costs of the resulting partition.

- *Might access frequencies change over time?* – Preordering a list or tree to exploit a skewed access pattern requires knowing the access pattern in advance. For many applications, it can be difficult to obtain such information. Better are *self-organizing lists*, where the order of the keys changes in response to the queries. The best self-organizing scheme is move-to-front; that is, we move the most recently searched-for key from its current position to the front of the list. Popular keys keep getting boosted to the front, while unsearched-for

keys drift towards the back of the list. There is no need to keep track of the frequency of access; just move the keys on demand. Self-organizing lists also exploit *locality of reference*, since accesses to a given key are likely to occur in clusters. A hot key will be maintained near the top of the list during a cluster of accesses, even if other keys have proven more popular in the past.

Self-organization can extend the useful size range of sequential search. However, you should switch to binary search beyond 100 elements. But consider using *splay trees*. which are self-organizing binary search trees that rotate each searched-for node to the root. They offer excellent amortized performance guarantees.

- *Is the key close by?* – Suppose we know that the target key is to the right of position p, and we think it is nearby. A sequential search is fast if we are correct, but we will be punished severely when we guess wrong. A better idea is to test repeatedly at larger intervals ($p+1$, $p+2$, $p+4$, $p+8$, $p+16$, ...) to the right until we find a key to the right of our target. Now we have a window containing the target and we can proceed with binary search.

  Such a *one-sided binary search* finds the target at position $p+l$ using at most $2\lceil \lg l \rceil$ comparisons, so it is faster than binary search when $l << n$, yet it can never be much worse. One-sided binary search is particularly useful in unbounded search problems, such as in numerical root finding.

- *Is my data structure sitting on external memory?* – Once the number of keys grows *too* large, a binary search loses its status as the best search technique. A binary search jumps wildly around the set of keys looking for midpoints to compare, and so each comparison requires reading a new page in from external memory. Much better are data structures such as B-trees (see Section 12.1 (page 367)) or Emde Boas trees (see notes below), which cluster the keys into pages to minimize the number of disk accesses per search.

- *Can I guess where the key should be?* – In *interpolation search*, we exploit our understanding of the distribution of keys to guess where to look next. An interpolation search is probably a more accurate description of how we use a telephone book than binary search. Suppose we are searching for *Washington, George* in a sorted telephone book. We would be safe making our first comparison three-fourths of the way down the list, essentially doing two comparisons for the price of one.

  Although an interpolation search is an appealing idea, we caution against it for three reasons: First, you have to work very hard to optimize your search algorithm before you can hope for a speedup over binary search. Second, even if you do beat a binary search, it is unlikely to be by enough to have justified the exercise. Finally, your program will be much less robust and efficient when the distribution changes, such as when your application gets ported to work on French words instead of English.

Implementations: The basic sequential and binary search algorithms are simple enough that you may consider implementing them yourself. That said, the C standard library contains `bsearch`, a generic implementation of (presumably) a binary search. The C++ *Standard Template Library* (STL) provides `find` (sequential search) and `binary_search` iterators. *Java Collections* (JC), provides `binarySearch` in the `java.util` package of Java standard edition (*http://java.sun.com/javase/*).

Many data structure textbooks provide extensive and illustrative implementations. Sedgewick (*http://www.cs.princeton.edu/∼rs/*) [Sed98] and Weiss (*http://www.cs.fiu.edu/∼weiss/*) [Wei06] provide implementation of splay trees and other search structures in both C++ and Java.

Notes: *The Handbook of Data Structures and Applications* [MS05] provides up-to-date surveys on all aspects of dictionary data structures. Other surveys include Mehlhorn and Tsakalidis [MT90b] and Gonnet and Baeza-Yates [GBY91]. Knuth [Knu97a] provides a detailed analysis and exposition on all fundamental search algorithms and dictionary data structures, but omits such modern data structures as red-black and splay trees.

The next position probed in linear interpolation search on an array of sorted numbers is given by

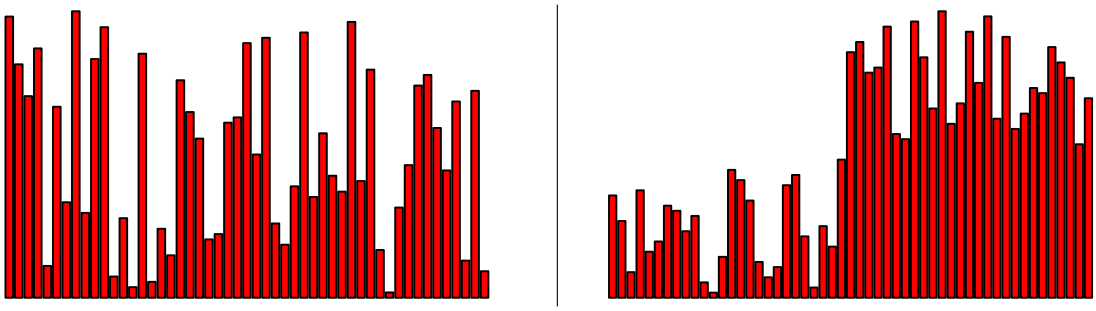
$$next = (low - 1) + \lceil \frac{q - S[low - 1]}{S[high + 1] - S[low - 1]} \times (high - low + 1) \rceil$$

where q is the query numerical key and S the sorted numerical array. If the keys are drawn independently from a uniform distribution, the expected search time is $O(\lg \lg n)$ [DJP04, PIA78].

Nonuniform access patterns can be exploited in binary search trees by structuring them so that popular keys are located near the root, thus minimizing search time. Dynamic programming can be used to construct such optimal search trees in $O(n \lg n)$ time [Knu98]. Stout and Warren [SW86b] provide a slick algorithm to efficiently transform a binary tree to a minimum height (optimally balanced) tree using rotations.

The Van Emde Boas layout of a binary tree (or sorted array) offers better external memory performance than conventional binary search, at a cost of greater implementation complexity. See the survey of Arge, et al. [ABF05] for more on this and other cache-oblivious data structures.

Related Problems: Dictionaries (see page 367), sorting (see page 436).



INPUT OUTPUT

14.3 Median and Selection

Input description: A set of n numbers or keys, and an integer k.

Problem description: Find the key smaller than exactly k of the n keys.

Discussion: Median finding is an essential problem in statistics, where it provides a more robust notion of average than the *mean*. The mean wealth of people who have published research papers on sorting is significantly affected by the presence of one William Gates [GP79], although his effect on the *median* wealth is merely to cancel out one starving graduate student.

Median finding is a special case of the more general *selection* problem, which asks for the kth element in sorted order. Selection arises in several applications:

- *Filtering outlying elements* – In dealing with noisy data, it is usually a good idea to throw out (say) the 10% largest and smallest values. Selection can be used to identify the items defining the 10^{th} and 90^{th} percentiles, and the outliers then filtered out by comparing each item to the two selected bounds.
- *Identifying the most promising candidates* – In a computer chess program, we might quickly evaluate all possible next moves, and then decide to study the top 25% more carefully. Selection followed by filtering is the way to go.
- *Deciles and related divisions* – A useful way to present income distribution in a population is to chart the salary of the people ranked at regular intervals, say exactly at the 10th percentile, 20th percentile, etc. Computing these values is simply selection on the appropriate position ranks.
- *Order statistics* – Particularly interesting special cases of selection include finding the smallest element ($k = 1$), the largest element ($k = n$), and the median element ($k = n/2$).

The mean of n numbers can be computed in linear time by summing the elements and dividing by n. However, finding the median is a more difficult problem. Algorithms that compute the median can readily be generalized to arbitrary selection. Issues in median finding and selection include:

- *How fast does it have to be?* – The most elementary median-finding algorithm sorts the items in $O(n \lg n)$ time and then returns the item occupying the $(n/2)$nd position. The good thing is that this gives much more information than just the median, enabling you to select the kth element (for any $1 \leq k \leq n$) in constant time after the sort. However, there are faster algorithms if all you want is the median.

  In particular, there is an $O(n)$ *expected*-time algorithm based on quicksort. Select a random element in the data set as a pivot, and use it to partition the data into sets of elements less than and greater than the pivot. From the sizes of these sets, we know the position of the pivot in the total order, and hence whether the median lies to the left or right of this point. Now we recur on the appropriate subset until it converges on the median. This takes (on average) $O(\lg n)$ iterations, with the cost of each iteration being roughly half that of the previous one. This defines a geometric series that converges to a linear-time algorithm, although if you are very unlucky it takes the same time as quicksort, $O(n^2)$.

  More complicated algorithms can find the median in worst-case linear time. However, the expected-time algorithm will likely win in practice. Just make sure to select random pivots to avoid the worst case.

- *What if you only get to see each element once?* – Selection and median finding become expensive on large datasets because they typically require several passes through external memory. In data-streaming applications, the volume of data is often too large to store, making repeated consideration (and thus exact median finding) impossible. Much better is computing a small summary of the data for future analysis, say approximate deciles or frequency moments (where the kth moment of stream x is defined as $F_k = \sum_i x_i^k$).

  One solution to such a problem is random sampling. Flip a coin for each value to decide whether to store it, with the probability of heads set low enough that you won't overflow your buffer. Likely the median of your samples will be close to that of the underlying data set. Alternately, you can devote some fraction of memory to retaining (say) decile values of large blocks, and then combine these decile distributions to yield more refined decile bounds.

- *How fast can you find the mode?* – Beyond mean and median lies a third notion of average. The *mode* is defined to be the element that occurs the greatest number of times in the data set. The best way to compute the mode sorts the set in $O(n \lg n)$ time, which places all identical elements next to each other. By doing a linear sweep from left to right on this sorted set, we can

count the length of the longest run of identical elements and hence compute the mode in a total of $O(n \lg n)$ time.

In fact, there is no faster worst-case algorithm possible to compute the mode, since the problem of testing whether there exist two identical elements in a set (called element uniqueness) can be shown to have an $\Omega(n \log n)$ lower bound. Element uniqueness is equivalent to asking whether the mode occurs more than once. Possibilities exist, at least theoretically, for improvements when the mode is large by using fast median computations.

Implementations: The C++ *Standard Template Library* (STL) provides a general selection method (`nth_element`) implemented using the linear expected-time algorithm. It is available with documentation at *http://www.sgi.com/tech/stl/*. See Josuttis [Jos99], Meyers [Mey01] and Musser [MDS01] for more detailed guides to using STL and the C++ standard library.

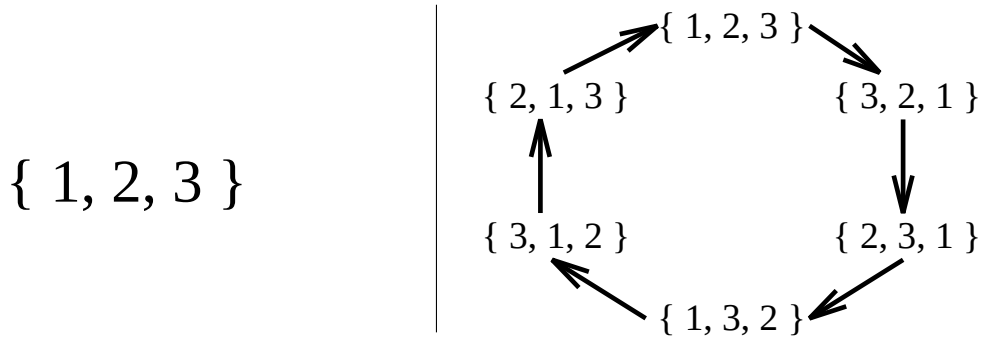
Notes: The linear expected-time algorithm for median and selection is due to Hoare [Hoa61]. Floyd and Rivest [FR75] provide an algorithm that uses fewer comparisons on average. Good expositions on linear-time selection include [AHU74, BvG99, CLRS01, Raw92], with [Raw92] being particularly enlightening.

Streaming algorithms have extensive applications to large data sets, and are well surveyed by Muthukrishnan [Mut05].

A sport of considerable theoretical interest is determining *exactly* how many comparisons are sufficient to find the median of n items. The linear-time algorithm of Blum et al. [BFP+72] proves that $c \cdot n$ suffice, but we want to know what c is. Dor and Zwick [DZ99] proved that $2.95n$ comparisons suffice to find the median. These algorithms attempt to minimize the number of element comparisons but not the total number of operations, and hence do not lead to faster algorithms in practice. They also hold the current best lower bower bound of $(2 + \epsilon)$ comparisons for median finding [DZ01].

Tight combinatorial bounds for selection problems are presented in [Aig88]. An optimal algorithm for computing the mode is given by [DM80].

Related Problems: Priority queues (see page 373), sorting (see page 436).



INPUT OUTPUT

14.4 Generating Permutations

Input description: An integer n.

Problem description: Generate (1) all, or (2) a random, or (3) the next permutation of length n.

Discussion: A permutation describes an arrangement or ordering of items. Many algorithmic problems in this catalog seek the best way to order a set of objects, including *traveling salesman* (the least-cost order to visit n cities), *bandwidth* (order the vertices of a graph on a line so as to minimize the length of the longest edge), and *graph isomorphism* (order the vertices of one graph so that it is identical to another). Any algorithm for solving such problems exactly must construct a series of permutations along the way.

There are $n!$ permutations of n items. This grows so quickly that you can't really expect to generate all permutations for $n > 12$, since $12! = 479{,}001{,}600$. Numbers like these should cool the ardor of anyone interested in exhaustive search and help explain the importance of generating random permutations.

Fundamental to any permutation-generation algorithm is a notion of order, the sequence in which the permutations are constructed from first to last. The most natural generation order is *lexicographic*, the sequence they would appear if they were sorted numerically. Lexicographic order for $n = 3$ is $\{1, 2, 3\}$, $\{1, 3, 2\}$, $\{2, 1, 3\}$, $\{2, 3, 1\}$, $\{3, 1, 2\}$, and finally $\{3, 2, 1\}$. Although lexicographic order is aesthetically pleasing, there is often no particular advantage to using it. For example, if you are searching through a collection of files, it does not matter whether the filenames are encountered in sorted order, so long as you eventually search through all of them. Indeed, nonlexicographic orders lead to faster and simpler permutation generation algorithms.

There are two different paradigms for constructing permutations: ranking/unranking and incremental change methods. The latter are more efficient, but ranking and unranking can be applied to solve a much wider class of problems. The key is to define the functions *rank* and *unrank* on all permutations p and integers n, m, where $|p| = n$ and $0 \leq m \leq n!$.

- *Rank(p)* – What is the position of p in the given generation order? A typical ranking function is recursive, such as basis case $Rank(\{1\}) = 0$ with

  $$Rank(p) = (p_1 - 1) \cdot (|p| - 1)! + Rank(p_2, \ldots, p_{|p|})$$

  Getting this right means relabeling the elements of the smaller permutation to reflect the deleted first element. Thus

  $$Rank(\{2, 1, 3\}) = 1 \cdot 2! + Rank(\{1, 2\}) = 2 + 0 \cdot 1! + Rank(\{1\}) = 2$$

- *Unrank(m,n)* – Which permutation is in position m of the $n!$ permutations of n items? A typical unranking function finds the number of times $(n-1)!$ goes into m and proceeds recursively. $Unrank(2, 3)$ tells us that the first element of the permutation must be '2', since $(2-1) \cdot (3-1)! \leq 2$ but $(3-1) \cdot (3-1)! > 2$. Deleting $(2-1) \cdot (3-1)!$ from m leaves the smaller problem $Unrank(0, 2)$. The ranking of 0 corresponds to the total order. The total order on the two remaining elements (since 2 has been used) is $\{1, 3\}$, so $Unrank(2, 3) = \{2, 1, 3\}$.

What the actual rank and unrank functions are does not matter as much as the fact that they must be inverses of each other. In other words, $p = Unrank(Rank(p), n)$ for all permutations p. Once you define ranking and unranking functions for permutations, you can solve a host of related problems:

- *Sequencing permutations* – To determine the *next* permutation that occurs in order after p, we can $Rank(p)$, add 1, and then $Unrank(p)$. Similarly, the permutation right before p in order is $Unrank(Rank(p) - 1, |p|)$. Counting through the integers from 0 to $n! - 1$ and unranking them is equivalent to generating all permutations.

- *Generating random permutations* – Selecting a random integer from 0 to $n!-1$ and then unranking it yields a truly random permutation.

- *Keep track of a set of permutations* – Suppose we want to construct random permutations and act only when we encounter one we have not seen before. We can set up a bit vector (see Section 12.5 (page 385)) with $n!$ bits, and set bit i to 1 if permutation *Unrank(i,n)* has been seen. A similar technique was employed with k-subsets in the Lotto application of Section 1.6 (page 23).

This rank/unrank method is best suited for small values of n, since $n!$ quickly exceeds the capacity of machine integers unless arbitrary-precision arithmetic is available (see Section 13.9 (page 423)). The incremental change methods work by defining the *next* and *previous* operations to transform one permutation into another, typically by swapping two elements. The tricky part is to schedule the swaps so that permutations do not repeat until all of them have been generated. The output picture above gives an ordering of the six permutations of $\{1, 2, 3\}$ using a single swap between successive permutations.

Incremental change algorithms for sequencing permutations are tricky, but they are so concise that they can be expressed in a dozen-line program. See the implementation section for pointers to code. Because the incremental change is only a single swap, these algorithms can be extremely fast—on average, constant time—which is independent of the size of the permutation! The secret is to represent the permutation using an n-element array to facilitate the swap. In certain applications, only the change between permutations is important. For example, in a brute-force program to search for the optimal TSP tour, the cost of the tour associated with the new permutation will be that of the previous permutation, with the addition and deletion of four edges.

Throughout this discussion, we have assumed that the items we are permuting are all distinguishable. However, if there are duplicates (meaning our set is a *multi-set*), you can save considerable time and effort by avoiding identical permutations. For example, there are only ten distinct permutations of $\{1, 1, 2, 2, 2\}$, instead of 120. To avoid duplicates, use backtracking and generate the permutations in lexicographic order.

Generating random permutations is an important little problem that people often stumble across, and often botch up. The right way is to use the following two-line, linear-time algorithm. We assume that *Random[i,n]* generates a random integer between i and n, inclusive.

for $i = 1$ to n do $a[i] = i$;
for $i = 1$ to $n - 1$ do $swap[a[i], a[Random[i, n]]$;

That this algorithm generates all permutations uniformly at random is not obvious. If you think so, convincingly explain why the following algorithm *does not* generate permutations uniformly:

for $i = 1$ to n do $a[i] = i$;
for $i = 1$ to $n - 1$ do $swap[a[i], a[Random[1, n]]$;

Such subtleties demonstrate why you must be very careful with random generation algorithms. Indeed, we recommend that you try some reasonably extensive experiments with *any* random generator before really believing it. For example, generate 10,000 random permutations of length 4 and see whether all 24 distinct permutations occur approximately the same number of times. If you know how to measure statistical significance, you are in even better shape.

Implementations: The C++ *Standard Template Library* (STL) provides two functions (`next_permutation` and `prev_permutation`) for sequencing permutations in lexicographic order. Kreher and Stinson [KS99] provide implementations of minimum change and lexicographic permutation generation in C at *http://www.math.mtu.edu/~kreher/cages/Src.html*.

The *Combinatorial Object Server* (*http://theory.cs.uvic.ca/*) developed by Frank Ruskey of the University of Victoria is a unique resource for generating permutations, subsets, partitions, graphs, and other objects. An interactive interface enables you to specify which objects you would like returned to you. Implementations in C, Pascal, and Java are available for certain types of objects.

C++ routines for generating an astonishing variety of combinatorial objects, including permutations and cyclic permutations, are available at *http://www.jjj.de/fxt/*.

Nijenhuis and Wilf [NW78] is a venerable but still excellent source on generating combinatorial objects. They provide efficient Fortran implementations of algorithms to construct random permutations and to sequence permutations in minimum-change order. Also included are routines to extract the cycle structure of a permutation. See Section 19.1.10 (page 661) for details.

Combinatorica [PS03] provides Mathematica implementations of algorithms that construct random permutations and sequence permutations in minimum change and lexicographic orders. It also provides a backtracking routine to construct all distinct permutations of a multiset, and it supports various permutation group operations. See Section 19.1.9 (page 661).

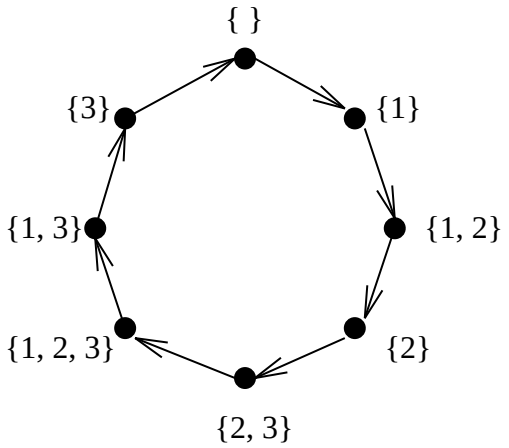
Notes: The best recent reference on permutation generation is Knuth [Knu05a]. Sedgewick's excellent survey on the topic is older [Sed77], but this is not a fast moving area. Good expositions include [KS99, NW78, Rus03].

Fast permutation generation methods make only a single swap between successive permutations. The Johnson-Trotter algorithm [Joh63, Tro62] satisfies an even stronger condition, namely that the two elements being swapped are always adjacent. Simple linear-time ranking and unranking functions for permutations are given by Myrvold and Ruskey [MR01].

In the days before ready access to computers, books with tables of random permutations [MO63] were used instead of algorithms. The swap-based random permutation algorithm presented above was first described in [MO63].

Related Problems: Random-number generation (see page 415), generating subsets (see page 452), generating partitions (see page 456).

{ 1, 2, 3 }



INPUT OUTPUT

14.5 Generating Subsets

Input description: An integer n.

Problem description: Generate (1) all, or (2) a random, or (3) the next subset of the integers $\{1, \ldots, n\}$.

Discussion: A subset describes a selection of objects, where the order among them does not matter. Many important algorithmic problems seek the best subset of a group of things: *vertex cover* seeks the smallest subset of vertices to touch each edge in a graph; *knapsack* seeks the most profitable subset of items of bounded total size; while *set packing* seeks the smallest subset of subsets that together cover each item exactly once.

There are 2^n distinct subsets of an n-element set, including the empty set as well as the set itself. This grows exponentially, but at a considerably slower rate than the $n!$ permutations of n items. Indeed, since $2^{20} = 1{,}048{,}576$, a brute-force search through all subsets of 20 elements is easily manageable. Since $2^{30} = 1{,}073{,}741{,}824$, you will certainly hit limits for slightly larger values of n.

By definition, the relative order among the elements does not distinguish different subsets. Thus, $\{1, 2, 5\}$ is the same as $\{2, 1, 5\}$. However, it is a very good idea to maintain your subsets in a sorted or *canonical* order to speed up such operations as testing whether or not two subsets are identical.

As with permutations (see Section 14.4 (page 448)), the key to subset generation problems is establishing a numerical sequence among all 2^n subsets. There are three primary alternatives:

- *Lexicographic order* – Lexicographic order means sorted order, and is often the most natural way to generate combinatorial objects. The eight subsets of $\{1, 2, 3\}$ in lexicographic order are $\{\}$, $\{1\}$, $\{1, 2\}$, $\{1, 2, 3\}$, $\{1, 3\}$, $\{2\}$, $\{2, 3\}$, and $\{3\}$. But it is surprisingly difficult to generate subsets in lexicographic order. Unless you have a compelling reason to do so, don't bother.

- *Gray Code* – A particularly interesting and useful subset sequence is the minimum change order, wherein adjacent subsets differ by the insertion or deletion of exactly one element. Such an ordering, called a *Gray code*, appears in the output picture above.

  Generating subsets in Gray code order can be very fast, because there is a nice recursive construction. Construct a Gray code of $n - 1$ elements G_{n-1}. Reverse a second copy of G_{n-1} and add n to each subset in this copy. Then concatenate them together to create G_n. Study the output example for clarification.

  Further, since only one element changes between subsets, exhaustive search algorithms built on Gray codes can be quite efficient. A set cover program would only have to update the change in coverage by the addition or deletion of one subset. See the implementation section below for Gray code subset-generation programs.

- *Binary counting* – The simplest approach to subset-generation problems is based on the observation that any subset S' is defined by the items of that S are in S'. We can represent S' by a binary string of n bits, where bit i is 1 iff the ith element of S is in S'. This defines a bijection between the 2^n binary strings of length n, and the 2^n subsets of n items. For $n = 3$, binary counting generates subsets in the following order: {}, {3}, {2}, {2,3}, {1}, {1,3}, {1,2}, {1,2,3}.

  This binary representation is the key to solving all subset generation problems. To generate all subsets in order, simply count from 0 to $2^n - 1$. For each integer, successively mask off each of the bits and compose a subset of exactly the items corresponding to 1 bits. To generate the *next* or *previous* subset, increment or decrement the integer by one. *Unranking* a subset is exactly the masking procedure, while *ranking* constructs a binary number with 1's corresponding to items in S and then converts this binary number to an integer.

  To generate a random subset, you might generate a random integer from 0 to $2^n - 1$ and unrank, although how your random number generator rounds things off might mean that certain subsets can never occur. Much better is to flip a coin n times, with the ith flip deciding whether to include element i in the subset. A coin flip can be robustly simulated by generating a random real or large integer and testing whether it is bigger or smaller than half its range. A Boolean array of n items can thus be used to represent subsets as a sort of premasked integer.

Generation problems for two closely related problems arise often in practice:

- *K-subsets* – Instead of constructing all subsets, we may only be interested in the subsets containing exactly k elements. There are $\binom{n}{k}$ such subsets, which is substantially less than 2^n, particularly for small values of k.

  The best way to construct all k-subsets is in lexicographic order. The ranking function is based on the observation that there are $\binom{n-f}{k-1}$ k-subsets whose smallest element is f. Using this, it is possible to determine the smallest element in the mth k-subset of n items. We then proceed recursively for subsequent elements of the subset. See the implementations below for details.

- *Strings* – Generating all subsets is equivalent to generating all 2^n strings of true and false. The same basic techniques apply to generate all or random strings on alphabets of size α, except there will be α^n strings in total.

Implementations: Kreher and Stinson [KS99] provide generators for both subsets and k-subsets, including lexicographic and Gray code orders. These implementations in C are available at *http://www.math.mtu.edu/~kreher/cages/Src.html*.

The *Combinatorial Object Server* (*http://theory.cs.uvic.ca/*), developed by Frank Ruskey of the University of Victoria, is a unique resource for generating permutations, subsets, partitions, graphs, and other objects. An interactive interface enables you to specify which objects you would like returned to you. Implementations in C, Pascal, and Java are available for certain types of objects.

C++ routines for generating an astonishing variety of combinatorial objects, including subsets and k-subsets (combinations), are available in the combinatorics package at *http://www.jjj.de/fxt/*.

Nijenhuis and Wilf [NW78] is a venerable but still excellent source on generating combinatorial objects. They provide efficient Fortran implementations of algorithms to construct random subsets and to sequence subsets in Gray code and lexicographic order. They also provide routines to construct random k-subsets and sequence them in lexicographic order. See Section 19.1.10 (page 661) for details on ftp-ing these programs. Algorithm 515 [BL77] of the *Collected Algorithms of the ACM* is another Fortran implementation of lexicographic k-subsets, available from Netlib (see Section 19.1.5 (page 659)).

Combinatorica [PS03] provides Mathematica implementations of algorithms to construct random subsets and sequence subsets in Gray code, binary, and lexicographic order. They also provide routines to construct random k-subsets and strings, and sequence them lexicographically. See Section 19.1.9 (page 661) for further information on Combinatorica.

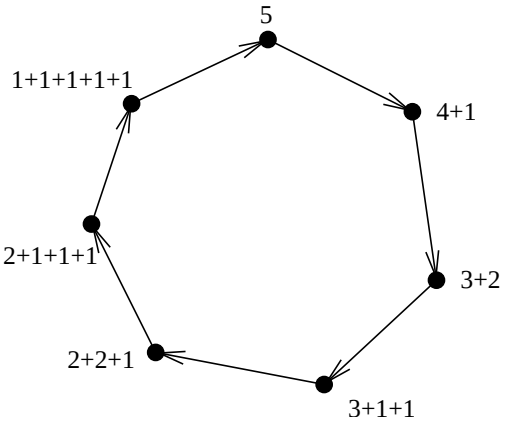
Notes: The best reference on subset generation is Knuth [Knu05b]. Good expositions include [KS99, NW78, Rus03]. Wilf [Wil89] provides an update of [NW78], including a thorough discussion of modern Gray code generation problems.

Gray codes were first developed [Gra53] to transmit digital information in a robust manner over an analog channel. By assigning the code words in Gray code order, the ith word differs only slightly from the $(i+1)$st, so minor fluctuations in analog signal strength corrupts only a few bits. Gray codes have a particularly nice correspondence to Hamiltonian cycles on the hypercube. Savage [Sav97] gives an excellent survey of Gray codes (minimum change orderings) for a large class of combinatorial objects, including subsets.

The popular puzzle *Spinout*, manufactured by ThinkFun (formerly Binary Arts Corporation), is solved using ideas from Gray codes.

Related Problems: Generating permutations (see page 448), generating partitions (see page 456).

N = 5



INPUT OUTPUT

14.6 Generating Partitions

Input description: An integer n.

Problem description: Generate (1) all, or (2) a random, or (3) the next integer or set partitions of length n.

Discussion: There are two different types of combinatorial objects denoted by the word "partition," namely integer partitions and set partitions. They are quite different beasts, but it is a good idea to make both a part of your vocabulary:

- *Integer partitions* are multisets of nonzero integers that add up exactly to n. For example, the seven distinct integer partitions of 5 are {5}, {4,1}, {3,2}, {3,1,1}, {2,2,1}, {2,1,1,1}, and {1,1,1,1,1}. An interesting application I encountered that required generating integer partitions was in a simulation of nuclear fission. When an atom is smashed, the nucleus of protons and neutrons is broken into a set of smaller clusters. The sum of the particles in the set of clusters must equal the original size of the nucleus. As such, the integer partitions of this original size represent all the possible ways to smash an atom.

- *Set partitions* divide the elements $1, \ldots, n$ into nonempty subsets. There are 15 distinct set partitions of $n = 4$: {1234}, {123,4}, {124,3}, {12,34}, {12,3,4}, {134,2}, {13,24}, {13,2,4}, {14,23}, {1,234}, {1,23,4}, {14,2,3}, {1,24,3}, {1,2,34}, and {1,2,3,4}. Several algorithm problems return set partitions as results, including *vertex/edge coloring* and *connected components*.

Although the number of integer partitions grows exponentially with n, they do so at a refreshingly slow rate. There are only 627 partitions of $n = 20$. It is even possible to enumerate all integer partitions of $n = 100$, since there there are only 190,569,292 of them.

The easiest way to generate integer partitions is to construct them in lexicographically decreasing order. The first partition is $\{n\}$ itself. The general rule is to subtract 1 from the smallest part that is > 1 and then collect all the 1's so as to match the new smallest part > 1. For example, the partition following $\{4, 3, 3, 3, 1, 1, 1, 1\}$ is $\{4, 3, 3, 2, 2, 2, 1\}$, since the five 1's left after $3 - 1 = 2$ becomes the smallest part are best packaged as 2,2,1. When the partition is all 1's, we have completed one pass through all the partitions.

This algorithm is sufficiently intricate to program that you should consider using one of the implementations below. In either case, test it to make sure that you get exactly 627 distinct partitions for $n = 20$.

Generating integer partitions uniformly at random is a trickier business than generating random permutations or subsets. This is because selecting the first (i.e. largest) element of the partition has a dramatic effect on the number of possible partitions that can be generated. Observe that no matter how large n is, there is only one partition of n whose largest part is 1. The number of partitions of n with largest part at most k is given by the recurrence

$$P_{n,k} = P_{n-k,k} + P_{n,k-1}$$

with the two boundary conditions $P_{x-y,x} = P_{x-y,x-y}$ and $P_{n,1} = 1$. This function can be used to select the largest part of your random partition with the correct probabilities and, by proceeding recursively, to eventually construct the entire random partition. Implementations are cited below.

Random partitions tend to have large numbers of fairly small parts, best visualized by a Ferrers diagram as in Figure 14.1. Each row of the diagram corresponds to one part of the partition, with the size of each part represented by that many dots.

Set partitions can be generated using techniques akin to integer partitions. Each set partition is encoded as a *restricted growth function*, $a_1, \ldots, a_n$, where $a_1 = 0$ and $a_i \leq 1 + \max(a_1, \ldots, a_i)$, for $i = 2, \ldots, n$. Each distinct digit identifies a subset, or *block*, of the partition, while the growth condition ensures that the blocks are sorted into a canonical order based on the smallest element in each block. For example, the restricted growth function $0, 1, 1, 2, 0, 3, 1$ defines the set partition $\{\{1, 5\}, \{2, 3, 7\}, \{4\}, \{6\}\}$.

Since there is a one-to-one equivalence between set partitions and restricted growth functions, we can use lexicographic order on the restricted growth functions to order the set partitions. Indeed, the fifteen partitions of $\{1, 2, 3, 4\}$ listed above are sequenced according to the lexicographic order of their restricted growth function (check it out).

We can use a similar counting strategy to generate random set partitions as we did with integer partitions. The Stirling numbers of the second kind $\{{n \atop k}\}$ count the

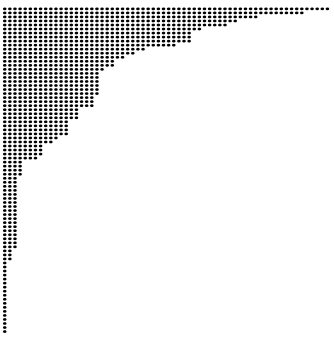


Figure 14.1: The Ferrers diagram of a random partition of $n = 1000$

number of partitions of $\{1, \ldots, n\}$ with exactly k blocks. They are computed using the recurrence

$$\left\{ {n \atop k} \right\} = \left\{ {n-1 \atop k-1} \right\} + k \left\{ {n-1 \atop k} \right\}$$

with the boundary conditions $\left\{ {n \atop n} \right\} = \left\{ {n \atop 1} \right\} = 1$. The reader is referred to the Notes and Implementations section for more details.

Implementations: Kreher and Stinson [KS99] generate both integer and set partitions in lexicographic order, including ranking/unranking functions. These implementations in C are available at *http://www.math.mtu.edu/~kreher/cages/Src.html*.

The *Combinatorial Object Server* (*http://theory.cs.uvic.ca/*) developed by Frank Ruskey of the University of Victoria is a unique resource for generating permutations, subsets, partitions, graphs, and other objects. An interactive interface enables you to specify which objects you would like returned. Implementations in C, Pascal, and Java are available for certain types of objects.

C++ routines for generating an astonishing variety of combinatorial objects, including integer partitions and compositions, are available in the combinatorics package at *http://www.jjj.de/fxt/*.

Nijenhuis and Wilf [NW78] is a venerable but still excellent source on generating combinatorial objects. They provide efficient Fortran implementations of algorithms to construct random and sequential integer partitions, set partitions, compositions, and Young tableaux. See Section 19.1.10 (page 661) for details.

Combinatorica [PS03] provides Mathematica implementations of algorithms to construct random and sequential integer partitions, compositions, strings, and

Young tableaux, as well as to count and manipulate these objects. See Section 19.1.9 (page 661).

Notes: The best reference on algorithms for generating both integer and set partitions is Knuth [Knu05b]. Good expositions include [KS99, NW78, Rus03, PS03]. Andrews [And98] is the primary reference on integer partitions and related topics, with [AE04] his more accessible introduction.

Integer and set partitions are both special cases of *multiset partitions*, or set partitions of nonnecessarily distinct numbers. In particular, the distinct set partitions on the multiset $\{1, 1, 1, \ldots, 1\}$ correspond exactly to integer partitions. Multiset partitions are discussed in Knuth [Knu05b].

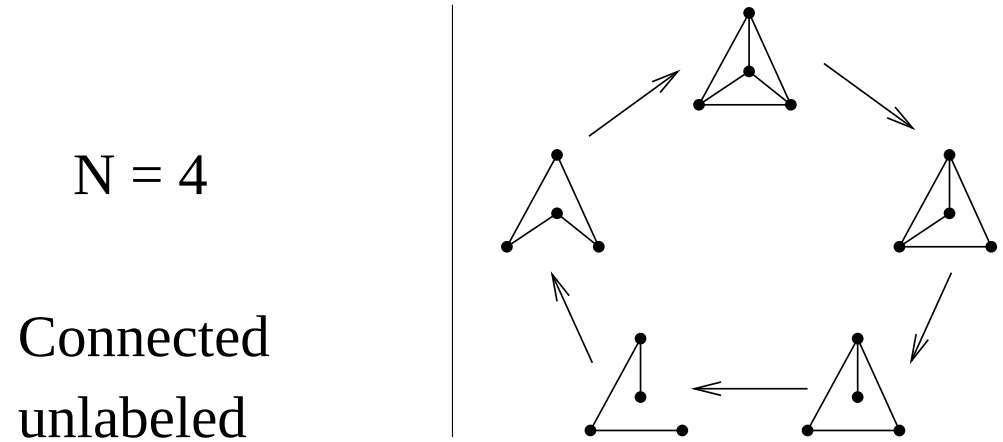
The (long) history of combinatorial object generation is detailed by Knuth [Knu06]. Particularly interesting are connections between set partitions and a Japanese incense burning game, and the naming of all 52 set partitions for $n = 5$ with distinct chapters from the oldest novel known, *The Tale of Genji*.

Two related combinatorial objects are Young tableaux and integer compositions, although they are less likely to emerge in applications. Generation algorithms for both are presented in [NW78, Rus03, PS03].

Young tableaux are two-dimensional configurations of integers $\{1, \ldots, n\}$ where the number of elements in each row is defined by an integer partition of n. Further, the elements of each row and column are sorted in increasing order, and the rows are left-justified. This notion of shape captures a wide variety of structures as special cases. They have many interesting properties, including the existence of a bijection between pairs of tableaux and permutations.

Compositions represent the possible assignments of a set of n indistinguishable balls to k distinguishable boxes. For example, we can place three balls into two boxes as {3,0}, {2,1}, {1,2}, or {0,3}. Compositions are most easily constructed sequentially in lexicographic order. To construct them randomly, pick a random $(k-1)$-subset of $n+k-1$ items using the algorithm of Section 14.5 (page 452), and count the number of unselected items between the selected ones. For example, if $k = 5$ and $n = 10$, the $(5-1)$ subset {1,3,7,14} of $1, \ldots, (n+k-1) = 14$ defines the composition {0,1,3,6,0}, since there are no items to the left of element 1 nor right of element 14.

Related Problems: Generating permutations (see page 448), generating subsets (see page 452).



INPUT OUTPUT

14.7 Generating Graphs

Input description: Parameters describing the desired graph, including the number of vertices n, and the number of edges m or edge probability p.

Problem description: Generate (1) all, or (2) a random, or (3) the next graph satisfying the parameters.

Discussion: Graph generation typically arises in constructing test data for programs. Perhaps you have two different programs that solve the same problem, and you want to see which one is faster or make sure that they always give the same answer. Another application is experimental graph theory, verifying whether a particular property is true for all graphs or how often it is true. It is much easier to believe the four-color theorem after you have demonstrated four colorings for all planar graphs on 15 vertices.

A different application of graph generation arises in network design. Suppose you need to design a network linking ten machines using as few cables as possible, such that this network can survive up to two vertex failures. One approach is to test all the networks with a given number of edges until you find one that will work. For larger graphs, heuristic approaches like simulated annealing will likely be necessary.

Many factors complicate the problem of generating graphs. First, make sure you know exactly what types of graphs you want to generate. Figure 5.2 on page 147 illustrates several important properties of graphs. For purposes of generation, the most important questions are:

- *Do I want labeled or unlabeled graphs?* – The issue here is whether the names of the vertices matter in deciding whether two graphs are the same. In generating *labeled graphs*, we seek to construct all possible labelings of all possible graph topologies. In generating *unlabeled graphs*, we seek only one representative for each topology and ignore labelings. For example, there are only two connected unlabeled graphs on three vertices—a triangle and a simple path. However, there are four connected labeled graphs on three vertices—one triangle and three 3-vertex paths, each distinguished by the name of their central vertex. In general, labeled graphs are much easier to generate. However, there are so many more of them that you quickly get swamped with isomorphic copies of the same few graphs.

- *Do I want directed or undirected graphs?* – Most natural generation algorithms generate undirected graphs. These can be turned into directed graphs by flipping coins to orient the edges. Any graph can be oriented to be directed and acyclic (i.e. , a DAG) by randomly permuting the vertices on a line and aiming each edge from left to right. With all such ideas, careful thought must be given to decide whether you are generating all graphs uniformly at random, and how much this matters to you.

You also must define what you mean by random. There are three primary models of random graphs, all of which generate graphs according to different probability distributions:

- *Random edge generation* – The first model is parameterized by a given edge probability p. Typically, $p = 0.5$, although smaller values can be used to construct sparser random graphs. In this model, a coin is flipped for each pair of vertices x and y to decide whether to add an edge (x, y). All *labeled* graphs will be generated with equal probability when $p = 1/2$.

- *Random edge selection* – The second model is parameterized by the desired number of edges m. It selects m distinct edges uniformly at random. One way to do this is by drawing random (x, y)-pairs and creating an edge if that pair is not already in the graph. An alternative approach to computing the same things constructs the set of $\binom{n}{2}$ possible edges and selects a random m-subset of them, as discussed in Section 14.5 (page 452).

- *Preferential attachment* – Under a rich-get-richer model, newly created edges are likely to point to high-degree vertices than low-degree ones. Consider new links (edges) being added to the graph of webpages. Under any realistic web generation model, it is much more likely the next link will be to Google than *http://www.cs.sunysb.edu/∼algorith.*[1] Selecting the next neighbor with

[1]Please link to us from your homepage to correct for this travesty.

probability proportional to its degree yields graphs with *power law* properties encountered in many real networks.

Which of these options best models your application? Probably none of them. Random graphs have very little structure by definition. But graphs are used to model relationships, which are often highly structured. Experiments conducted on random graphs, although interesting and easy to perform, often fail to capture what you are looking for.

An alternative to random graphs is "organic" graphs—graphs that reflect the relationships among real-world objects. The Stanford GraphBase, discussed below, is an outstanding source of organic graphs. Many raw sources of relationships are available on the web that can be turned into interesting organic graphs with a little programming and imagination. Consider the graph defined by a set of web-pages, with any hyperlink between two pages defining an edge. Or, what about the graph implicit in railroad, subway, or airline networks, with vertices being stations and edges between two stations connected by direct service? As a final example, every large computer program defines a call graph, where the vertices represent subroutines, and there is an edge (x, y) if x calls y.

Two classes of graphs have particularly interesting generation algorithms:

- *Trees* – Prüfer codes provide a simple way to rank and unrank *labeled* trees and thus solve all standard generation problems (see Section 14.4 (page 448)). There are exactly n^{n-2} labeled trees on n vertices, and exactly that many strings of length $n-2$ on the alphabet $\{1, 2, \ldots, n\}$.

  The key to Prüfer's bijection is the observation that every tree has at least two vertices of degree 1. Thus, in any labeled tree the vertex v incident on the leaf with lowest label is well defined. We take v to be S_1, the first character in the code. We then delete the associated leaf and repeat the procedure until only two vertices are left. This defines a unique code S for any given labeled tree that can be used to rank the tree. To go from code to tree, observe that the degree of vertex v in the tree is one more than the number of times v occurs in S. The lowest-labeled leaf will be the smallest integer missing from S, which when paired with S_1 determines the first edge of the tree. The entire tree follows by induction.

  Algorithms for efficiently generating unlabeled rooted trees are discussed in the Implementation section.

- *Fixed degree sequence graphs* – The *degree sequence* of a graph G is an integer partition $p = (p_1, \ldots, p_n)$, where p_i is the degree of the ith highest-degree vertex of G. Since each edge contributes to the degree of two vertices, p is an integer partition of $2m$, where m is the number of edges in G.

  Not all partitions correspond to degree sequences of graphs. However, there is a recursive construction that constructs a graph with a given degree sequence if one exists. If a partition is realizable, the highest-degree vertex v_1 can be

connected to the next p_1 highest-degree vertices in G, or the vertices corresponding to parts $p_2, \ldots, p_{p_1+1}$. Deleting p_1 and decrementing $p_2, \ldots, p_{p_1+1}$ yields a smaller partition, which we recur on. If we terminate without ever creating negative numbers, the partition was realizable. Since we always connect the highest-degree vertex to other high-degree vertices, it is important to reorder the parts of the partition by size after each iteration.

Although this construction is deterministic, a semi-random collection of graphs realizing this degree sequence can be generated from G using *edge-flipping* operations. Suppose edges (x, y) and (w, z) are in G, but (x, w) and (y, z) are not. Exchanging these pairs of edges creates a different (not necessarily connected) graph without changing the degrees of any vertex.

Implementations: The Stanford GraphBase [Knu94] is perhaps most useful as an instance generator for constructing graphs to serve as test data for other programs. It incorporates graphs derived from interactions of characters in famous novels, Roget's Thesaurus, the Mona Lisa, expander graphs, and the economy of the United States. It also contains routines for generating binary trees, graph products, line graphs, and other operations on basic graphs. Finally, because of its machine-independent, random-number generators, it provides a way to construct random graphs such that they can be reconstructed elsewhere, thus making them perfect for experimental comparisons of algorithms. See Section 19.1.8 (page 660) for additional information.

Combinatorica [PS03] provides Mathematica generators for such graphs as stars, wheels, complete graphs, random graphs and trees, and graphs with a given degree sequence. Further, it includes operations to construct more interesting graphs from these, including join, product, and line graph.

The *Combinatorial Object Server* (*http://theory.cs.uvic.ca/*) developed by Frank Ruskey of the University of Victoria provides routines for generating both free and rooted trees.

Viger [VL05] has made available a C++ implementation of his algorithm to generate simple connected graphs with a prescribed degree sequence. See *http://www.liafa.jussieu.fr/~fabien/generation/*.

The graph isomorphism testing program Nauty (see Section 16.9 (page 550)) includes a suite of programs for generating nonisomorphic graphs, plus special generators for bipartite graphs, digraphs, and multigraphs. They are available at *http://cs.anu.edu.au/~bdm/nauty/*.

The mathematicians Brendan McKay (*http://cs.anu.edu.au/~bdm/data/*) and Gordon Royle (*http://people.csse.uwa.edu.au/gordon/data.html*) provide exhaustive catalogs of several families of graphs and trees up to the largest reasonable number of vertices.

Nijenhuis and Wilf [NW78] provide efficient Fortran routines to enumerate all labeled trees via Prüfer codes and to construct random unlabeled rooted trees. See Section 19.1.10 (page 661). Kreher and Stinson [KS99] generate labeled trees in C,

with implementations available at *http://www.math.mtu.edu/~kreher/cages/Src.html*.

Notes: Extensive literature exists on generating graphs uniformly at random. Surveys include [Gol93, Tin90]. Closely related to the problem of generating classes of graphs is counting them. Harary and Palmer [HP73] survey results in graphical enumeration.

Knuth [Knu06] is the best recent reference on generating trees. The bijection between $n-2$ strings and labeled trees is due to Prüfer [Prü18].

Random graph theory is concerned with the properties of random graphs. Threshold laws in random graph theory define the edge density at which properties such as connectedness become highly likely to occur. Expositions on random graph theory include [Bol01, JLR00].

The preferential attachment model of graphical evolution has emerged relatively recently in the study of networks. See [Bar03, Wat04] for introductions to this exciting field.

An integer partition is *graphic* if there exists a simple graph with that degree sequence. Erdős and Gallai [EG60] proved that a degree sequence is graphic if and only if the sequence observes the following condition for each integer $r < n$:

$$\sum_{i=1}^{r} d_i \leq r(r-1) + \sum_{i=r+1}^{n} \min(r, d_i)$$

Related Problems: Generating permutations (see page 448), graph isomorphism (see page 550).

INPUT	OUTPUT
December 21, 2012 ? (Gregorian)	5773 Teveth 8 (Hebrew) 1434 Safar 7 (Islamic) 1934 Agrahayana 30 (Indian Civil) 13.0.0.0 (Mayan Long Count)

14.8 Calendrical Calculations

Input description: A particular calendar date d, specified by month, day, and year.

Problem description: Which day of the week did d fall on according to the given calendar system?

Discussion: Many business applications need to perform calendrical calculations. Perhaps we want to display a calendar of a specified month and year. Maybe we need to compute what day of the week or year some event occurs, as in figuring out the date on which a 180-day futures contract comes due. The importance of correct calendrical calculations was perhaps best revealed by the furor over the "Millennium bug"—the year 2000 crisis in legacy programs that allocated only two digits for storing the year.

More complicated questions arise in international applications, because different nations and ethnic groups use different calendar systems. Some of these, like the Gregorian calendar used in most of the world, are based on the Sun, while others, like the Hebrew calendar, are lunar calendars. How would you tell today's date according to the Chinese or Islamic calendar?

Calendrical calculations differ from other problems in this book because calendars are historical objects, not mathematical ones. The algorithmic issues revolve around specifying the rules of the calendrical system and implementing them correctly, rather than designing efficient shortcuts for the computation.

The basic approach underlying calendar systems is to start with a particular reference date (called the *epoch*) and count up from there. The particular rules for wrapping the count around into months and years is what distinguishes one system from another. Implementing a calendar requires two functions, one that, given a date, returns the integer number of days that have elapsed since the epoch, the other of which takes an integer n and returns the calendar date exactly n days

from epoch. These are exactly analogous to the ranking and unranking rules for combinatorial objects such as permutations (see Section 14.4 (page 448)).

That the solar year is not an integer number of days long is the major source of complications in calendar systems. To keep a calendar's annual dates in sync with the seasons, leap days must be added at both regular and irregular intervals. Since a solar year is 365 days and 5:49:12 hours long, adding a leap day every four years leaves an extra 10 minutes and 48 seconds unaccounted for each year.

The original Julian calendar (from Julius Caesar) ignored these extra minutes, which had accumulated to ten days by 1582. Pope Gregory XIII then proposed the Gregorian calendar used today, by deleting the ten days and eliminating leap days in years that are multiples of 100 but not 400. Supposedly, riots ensued because the masses feared their lives were being shortened by ten days. Outside the Catholic church, resistance to change slowed the reforms. The deletion of days did not occur in England and America until September 1752, and not until 1927 in Turkey.

The rules for most calendrical systems are sufficiently complicated and pointless that you should lift code from a reliable place rather than attempt to write your own. We identify suitable implementations next.

There are a variety of "impress your friends" algorithms that enable you to compute in your head what day of the week a particular date occurred. Such algorithms often fail to work reliably outside the given century and certainly should be avoided for computer implementation.

Implementations: Readily available calendar libraries exist in both C++ and Java. The Boost time-data library provides a reliable implementation of the Gregorian calendar in C++. See *http://www.boost.org/doc/html/date_time.html*. The Calendar class in `java.util.Calendar` implements the Gregorian calendar in Java. Either of these will likely suffice for most applications.

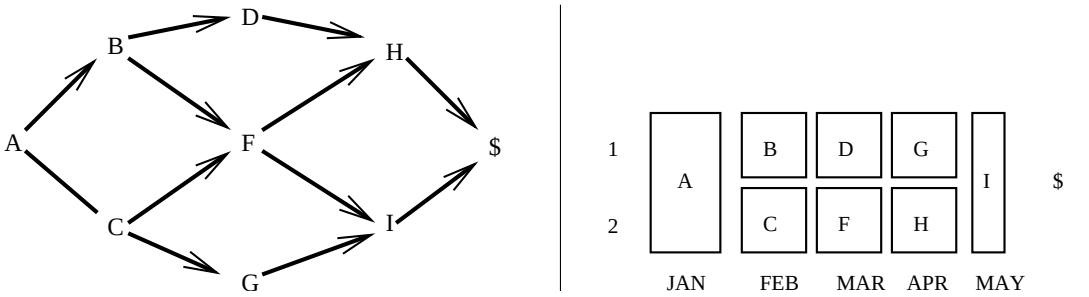
Dershowitz and Reingold provide a uniform algorithmic presentation [RD01] for a variety of different calendar systems, including the Gregorian, ISO, Chinese, Hindu, Islamic, and Hebrew calendars, as well as other calendars of historical interest. *Calendrical* is an implementation of these calendars in Common Lisp, Java, and Mathematica, with routines to convert dates between calendars, day of the week computations, and the determination of secular and religious holidays. *Calendrical* is likely to be the most comprehensive and reliable calendrical routines available. See their website at *http://calendarists.com*.

C and Java implementations of international calendars of unknown reliability are readily available at SourceForge (*http://sourceforge.net*). Search for "Gregorian calendar" to avoid the mass of datebook implementations.

Notes: A comprehensive discussion of calendrical computation algorithms appear in the papers of Dershowitz and Reingold [DR90, RDC93], which have been superseded by their book [RD01] that outlines algorithms for no less than 25 international and historical calendars Three hundred years of calendars representing tabulations for all dates from 1900 to 2200 appear in [DR02].

Concern exists in certain quarters whether December 21, 2012 represents the end of the world. The argument rests on it being the date the Mayan calendar spins over to 13.0.0.0.0 after a 5,125 year cycle. The reader should rest assured, since I would never have devoted so much effort to writing this book were the world to be ending so imminently. The Mayan calendar is authoritatively described in [RD01].

Related Problems: Arbitrary-precision arithmetic (see page 423), generating permutations (see page 448).



INPUT OUTPUT

14.9 Job Scheduling

Input description: A directed acyclic graph $G = (V, E)$, where vertices represent jobs and edge (u, v) implies that task u must be completed before task v.

Problem description: What schedule of tasks completes the job using the minimum amount of time or processors?

Discussion: Devising a proper schedule to satisfy a set of constraints is fundamental to many applications. Mapping tasks to processors is a critical aspect of any parallel-processing system. Poor scheduling can leave all other machines sitting idle while one bottleneck task is performed. Assigning people-to-jobs, meetings-to-rooms, or courses-to-exam periods are all different examples of scheduling problems.

Scheduling problems differ widely in the nature of the constraints that must be satisfied and the type of schedule desired. Several other catalog problems have application to various kinds of scheduling:

- Topological sorting can construct a schedule consistent with the precedence constraints. See Section 15.2 (page 481).
- Bipartite matching can assign a set of jobs to people who have the appropriate skills for them. See Section 15.6 (page 498).
- Vertex and edge coloring can assign a set of jobs to time slots such that no two interfering jobs are assigned the same time slot. See Sections 16.7 and 16.8.
- Traveling salesman can schedule select the most efficient route for a delivery person to visit a given set of locations. See Section 16.4 (page 533).

- Eulerian cycle can construct the most efficient route for a snowplow or mailman to completely traverse a given set of edges. See Section 15.7 (page 502).

Here we focus on precedence-constrained scheduling problems for directed acyclic graphs. Suppose you have broken a big job into a large number of smaller tasks. For each task, you know how long it should take (or perhaps an upper bound on how long it might take). Further, for each pair of tasks you know whether it is essential that one task be performed before the other. The fewer constraints we have to enforce, the better our schedule can be. These constraints must define a directed acyclic graph—acyclic because a cycle in the precedence constraints represents a Catch-22 situation that can never be resolved.

We are interested in several problems on these networks:

- *Critical path* – The longest path from the start vertex to the completion vertex defines the *critical path*. This can be important to know, for the only way to shorten the minimum total completion time is to reduce the time of one of the tasks on each critical path. The tasks on the critical paths can be determined in $O(n + m)$ time using the dynamic programming presented in Section 15.4 (page 489).

- *Minimum completion time* – What is the fastest we can get this job completed while respecting precedence constraints, assuming that we have an unlimited number of workers. If there were *no* precedence constraints, each task could be worked on by its own worker, and the total time would be that of the longest single task. If there are such strict precedence constraints that each task must follow the completion of its immediate predecessor, the minimum completion time would be obtained by summing up the times for each task.

  The minimum completion time for a DAG can be computed in $O(n+m)$ time. The completion time is defined by the critical path. To get such a schedule, consider the jobs in topological order, and start each job on a new processor the moment its latest prerequisite completes.

- *What is the tradeoff between the number of workers and completion time?* – What we really are interested in is how best to complete the schedule with a given number of workers. Unfortunately, this and most similar problems are NP-complete.

Any real scheduling application is likely to present combinations of constraints that will be difficult or impossible to model using these techniques. There are two reasonable ways to deal with such problems. First, we can ignore constraints until the problem reduces to one of the types that we have described here, solve it, and then see how bad it is with respect to the other constraints. Perhaps the schedule can be easily modified by hand to satisfy other esoteric constraints, like keeping Joe and Bob apart so they won't kill each other. Another approach is to formulate

your scheduling problem via linear-integer programming (see Section 13.6 (page 411)) in all its complexity. I always recommend starting out with something simple and see how it works before trying something complicated.

Another fundamental scheduling problem takes a set of jobs without precedence constraints and assigns them to identical machines to minimize the total elapsed time. Consider a copy shop with k Xerox machines and a stack of jobs to finish by the end of the day. Such tasks are called *job-shop scheduling*. They can be modeled as bin-packing (see Section 17.9 (page 595)), where each job is assigned a number equal to the number of hours it will take to complete, and each machine is represented by a bin with space equal to the number of hours in a day.

More sophisticated variations of job-shop scheduling provide each task with allowable start and required finishing times. Effective heuristics are known, based on sorting the tasks by size and finishing time. We refer the reader to the references for more information. Note that these scheduling problems become hard only when the tasks cannot be broken up onto multiple machines or interrupted (preempted) and then rescheduled. If your application allows these degrees of freedom, you should exploit them.

Implementations: JOBSHOP is a collection of C programs for job-shop scheduling created in the course of a computational study by Applegate and Cook [AC91]. They are available at *http://www2.isye.gatech.edu/∼wcook/jobshop/*.

Tablix (*http://tablix.org*) is an open source program for solving timetabling problems faced by real schools. Support for parallel/cluster computation is provided.

LEKIN is a flexible job-shop scheduling system designed for educational use [Pin02]. It supports single machine, parallel machines, flow-shop, flexible flow-shop, job-shop, and flexible job-shop scheduling, and is available at *http://www.stern.nyu.edu/om/software/lekin*.

For commercial scheduling applications, ILOG CP is reflective of the state-of-the-art. For more, see *http://www.ilog.com/products/cp/*.

Algorithm 520 [WBCS77] of the *Collected Algorithms of the ACM* is a Fortran code for multiple-resource network scheduling. It is available from Netlib (see Section 19.1.5 (page 659)).

Notes: The literature on scheduling algorithms is a vast one. Brucker [Bru07] and Pinedo [Pin02] provide comprehensive overviews of the field. The *Handbook of Scheduling* [LA04] provides an up-to-date collection of surveys on all aspects of scheduling.

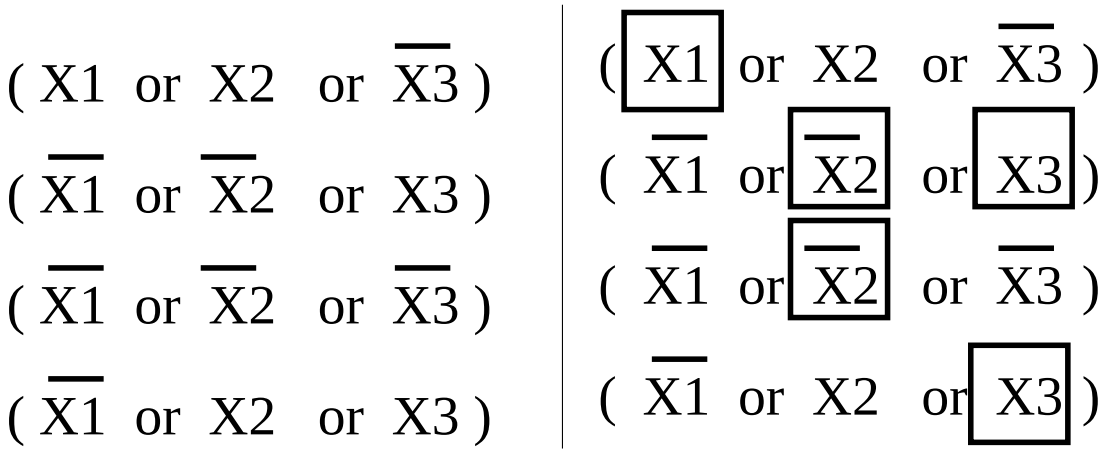
A well-defined taxonomy exists covering thousands of job-shop scheduling variants, which classifies each problem $\alpha|\beta|\gamma$ according to (α) the machine environment, (β) details of processing characteristics and constraints, and (γ) the objectives to be minimized. Surveys of results include [Bru07, CPW98, LLK83, Pin02].

Gantt charts provide visual representations of job-shop scheduling solutions, where the x-axis represents time and rows represent distinct machines. The output figure above illustrates a Gantt chart. Each scheduled job is represented as a horizontal block, thus identifying its start-time, duration, and server. Project precedence-constrained scheduling

techniques are often called PERT/CPM, for *Program Evaluation and Review Technique/Critical Path Method*. Both Gantt charts and PERT/CPM appear in most textbooks on operations research, including [Pin02].

Timetabling is a term often used in discussion of classroom and related scheduling problems. PATAT (for *Practice and Theory of Automated Timetabling*) is a biannual conference reporting new results in the field. Its proceedings are available from *http://www.asap.cs.nott.ac.uk/patat/patat-index.shtml*.

Related Problems: Topological sorting (see page 481), matching (see page 498), vertex coloring (see page 544), edge coloring (see page 548), bin packing (see page 595).



14.10 Satisfiability

Input description: A set of clauses in conjunctive normal form.

Problem description: Is there a truth assignment to the Boolean variables such that every clause is simultaneously satisfied?

Discussion: Satisfiability arises whenever we seek a configuration or object that must be consistent with (i.e. , satisfy) a set of logical constraints. A primary application is in verifying that a hardware or software system design works correctly on all inputs. Suppose a given logical formula $S(\bar{X})$ denotes the specified result on input variables $\bar{X} = X_1, \ldots, X_n$, while a different formula $C(\bar{X})$ denotes the Boolean logic of a proposed circuit for computing $S(\bar{X})$. This circuit is correct unless there exists an $\bar{X}$ such that $S(\bar{X}) \neq C(\bar{X})$.

Satisfiability (or SAT) is *the* original NP-complete problem. Despite its applications to constraint satisfaction, logic, and automatic theorem proving, it is perhaps most important theoretically as the root problem from which all other NP-completeness proofs originate. So much engineering has gone into today's best SAT solvers that they represent a reasonable starting point if one really needs to solve an NP-complete problem *exactly*. That said, employing heuristics that give good but nonoptimal solutions is usually the better approach in practice.

Issues in satisfiability testing include:

- *Is your formula the AND of ORs (CNF) or the OR of ANDs (DNF)?* – In satisfiability, constraints are specified as a logical formula. There are two

primary ways of expressing logical formulas—conjunctive normal form (CNF) and disjunctive normal form (DNF). In CNF formulas, we must satisfy all clauses, where each clause is constructed by and-ing or's of literals together, such as

$$(v_1 \text{ or } \bar{v_2}) \text{ and } (v_2 \text{ or } v_3)$$

In DNF formulas, we must satisfy any one clause, where each clause is constructed by or-ing ands of literals together. The formula above can be written in DNF as

$$(\bar{v_1} \text{ and } \bar{v_2} \text{ and } v_3) \text{ or } (\bar{v_1} \text{ and } v_2 \text{ and } \bar{v_3}) \text{ or } (\bar{v_1} \text{ and } v_2 \text{ and } v_3) \text{ or } (v_1 \text{ and } \bar{v_2} \text{ and } v_3)$$

Solving DNF-satisfiability is trivial, since any DNF formula can be satisfied unless *every* clause contains both a literal and its complement (negation). However, CNF-satisfiability is NP-complete. This seems paradoxical, since we can use De Morgan's laws to convert CNF-formulae into equivalent DNF-formulae, and vice versa. The catch is that an exponential number of terms might be constructed in the course of translation, so that the translation itself does not run in polynomial time.

- *How big are your clauses?* – k-SAT is a special case of satisfiability when each clause contains at most k literals. The problem of 1-SAT is trivial, since we must set true any literal appearing in any clause. The problem of 2-SAT is not trivial, but can still be solved in linear time. This is interesting, because certain problems can be modeled as 2-SAT using a little cleverness. The good times end as soon as clauses contain three literals each (i.e. , 3-SAT) for 3-SAT is NP-complete.

- *Does it suffice to satisfy* most *of the clauses?* – If you must solve it exactly, there is not much you can do to solve satisfiability except by backtracking algorithms such as the Davis-Putnam procedure. In the worst case, there are 2^m truth assignments to be tested, but fortunately there are many ways to prune the search. Although satisfiability is NP-complete, how hard it is in practice depends on how the instances are generated. Naturally defined "random" instances are often surprisingly easy to solve, and in fact it is nontrivial to generate instances of the problem that are truly hard.

  Still, we can benefit by relaxing the problem so that the goal becomes satisfying as many clauses as possible. Optimization techniques such as simulated annealing can then be put to work to refine random or heuristic solutions. Indeed, any random truth assignment to the variables will satisfy each k-SAT clause with probability $1 - (1/2)^k$, so our first attempt is likely to satisfy most of the clauses. Finishing off the job is the hard part. Finding an assignment that satisfies the maximum number of clauses is NP-complete even for nonsatisfiable instances.

When faced with a problem of unknown complexity, proving it NP-complete can be an important first step. If you think your problem might be hard, skim through Garey and Johnson [GJ79] looking for your problem. If you don't find it, I recommend that you put the book away and try to prove hardness from first principles, using the basic problems of 3-SAT, vertex cover, independent set, integer partition, clique, and Hamiltonian cycle. I find it much easier to start from these than some complicated problem in the book, and more insightful too, since the reason for the hardness is not obscured by the hidden hardness proof for the complicated problem. Chapter 9 focuses on strategies for proving hardness.

Implementations: Recent years have seen tremendous progress in the performance of SAT solvers. An annual SAT competition identifies the top performing solvers in each of three categories of instances (drawn from industrial, handmade, and random problem instances, respectively).

The top three programs of the SAT 2007 industrial competition were Rsat (*http://reasoning.cs.ucla.edu/rsat/*), PicoSAT (*http://fmv.jku.at/picosat/*) and MiniSAT (*http://www.cs.chalmers.se/Cs/Research/FormalMethods/MiniSat/*). The source code for all these solvers and more are available from the competition webpage (*http://www.satcompetition.org/*).

SAT *Live!* (*http://www.satlive.org/*) is the most up-to-date source for papers, programs, and test sets for satisfiability and related logic optimization problems.

Notes: The most comprehensive overview of satisfiability testing is Kautz, et al. [KSBD07]. The Davis-Putnam-Logemann-Loveland (DPLL) algorithm is a backtracking algorithm introduced in 1962 for solving satisfiability problems. Local search techniques work better on certain classes of problems that are difficult for DPLL solvers. *Chaff* [MMZ$^+$01] is a particularly influential solver, available at *http://www.princeton.edu/∼chaff/*. See [KS07] for a survey of recent progress in the field of satisfiability testing.

An algorithm for solving 3-SAT in worst-case $O^*(1.4802^n)$ appears in [DGH$^+$02]. Efficient (but nonpolynomial) algorithms for NP-complete problems are surveyed in [Woe03].

The primary reference on NP-completeness is [GJ79], featuring a list of roughly 400 NP-complete problems. The book remains an extremely useful reference; it is perhaps the book I reach for most often. An occasional column by David Johnson in the *Journal of Algorithms* and (now) *ACM Transactions on Algorithms* provides updates.

Good expositions of Cook's theorem [Coo71], where satisfiability is proven hard, include [CLRS01, GJ79, KT06]. The importance of Cook's result became clear in Karp's paper [Kar72], showing the hardness of over 20 different combinatorial problems.

A linear-time algorithm for 2-SAT appears in [APT79]. See [WW95] for an interesting application of 2-SAT to map labeling. The best heuristic known approximates maximum 2-SAT to within a factor of 1.0741 [FG95].

Related Problems: Constrained optimization (see page 407), traveling salesman problem (see page 533).

15

Graph Problems: Polynomial-Time

Algorithmic graph problems constitute approximately one third of the problems in this catalog. Problems from other sections could have been formulated equally well in terms of graphs, such as bandwidth minimization and finite-state automata optimization. Identifying the name of a graph-theoretic invariant or problem is one of the primary skills of a good algorist. Indeed, the catalog will tell you exactly how to proceed as soon as you figure out your particular problem's name.

In this section, we deal only with problems for which there are efficient algorithms to solve them. As there is often more than one way to model a given application, it makes sense to look here before proceeding on to the harder formulations.

The algorithms presented here have running times that grow polynomially with the size of the graph. We adopt throughout the convention that n refers to the number of vertices in a graph, while m is the number of edges.

Graphs are often best understood as drawings. Many interesting graph properties follow from the nature of a particular type of drawing, such as planar graphs. Thus, we also discuss algorithms for drawing graphs, trees, and planar graphs.

Most advanced graph algorithms are difficult to program. However, good implementations are available if you know where to look. The best general sources include LEDA [MN99] and the Boost Graph Library [SLL02]. However, better special-purpose codes exist for many problems.

See the *Handbook of Graph Algorithms* [TNX08] for up-to-date surveys on all areas of graph algorithms. Other excellent surveys include van Leeuwen [vL90a], and several chapters in Atallah [Ata98]. Books specializing in graph algorithms include:

- *Sedgewick* [Sed98] – The graph algorithms volume of this algorithms text provides a comprehensive but gentle introduction to the field.

S.S. Skiena, *The Algorithm Design Manual*, 2nd ed., DOI: 10.1007/978-1-84800-070-4_15,
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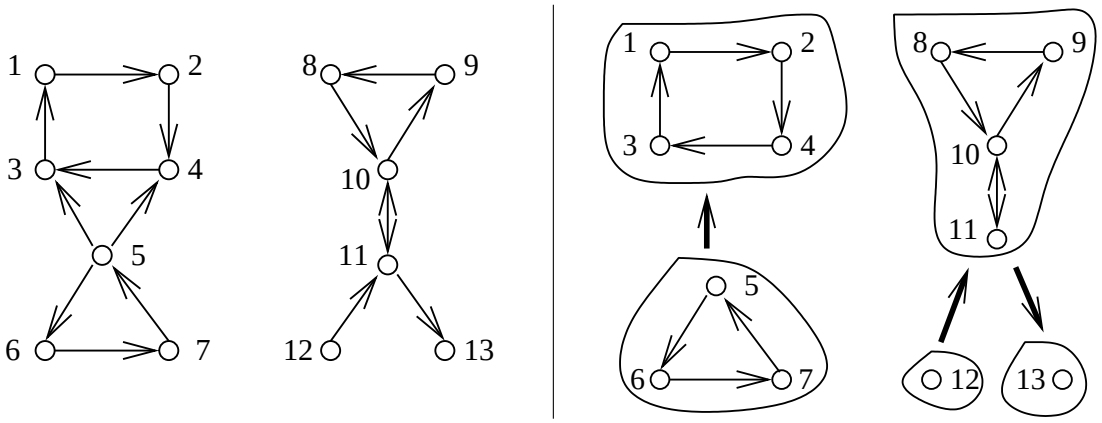
- *Ahuja, Magnanti, and Orlin* [AMO93] – While purporting to be a book on network flows, it covers the gamut of graph algorithms with an emphasis on operations research. Strongly recommended.
- *Gibbons* [Gib85] – A good book on graph algorithms, including planarity testing, matching, and Eulerian/Hamiltonian cycles, as well as more elementary topics.
- *Even* [Eve79a] – An older but still respected advanced text on graph algorithms, with a particularly thorough treatment of planarity-testing algorithms.



INPUT OUTPUT

15.1 Connected Components

Input description: A directed or undirected graph G.

Problem description: Identify the different pieces or components of G, where vertices x and y are members of different components if no path exists from x to y in G.

Discussion: The connected components of a graph represent, in grossest terms, the pieces of the graph. Two vertices are in the same component of G if and only if there exists some path between them.

Finding connected components is at the heart of many graph applications. For example, consider the problem of identifying natural clusters in a set of items. We represent each item by a vertex and add an edge between each pair of items deemed "similar." The connected components of this graph correspond to different classes of items.

Testing whether a graph is connected is an essential preprocessing step for every graph algorithm. Subtle, hard-to-detect bugs often result when an algorithm is run only on one component of a disconnected graph. Connectivity tests are so quick and easy that you should always verify the integrity of your input graph, even when you know for certain that it *has* to be connected.

Testing the connectivity of any undirected graph is a job for either depth-first or breadth-first search, as discussed in Section 5 (page 145). Which one you choose doesn't really matter. Both traversals initialize the *component-number* field for each vertex to 0, and then start the search for component 1 from vertex v_1. As each vertex is discovered, the value of this field is set to the current component

number. When the initial traversal ends, the component number is incremented, and the search begins again from the first vertex whose *component-number* remains 0. Properly implemented using adjacency lists (as is done in Section 5.7.1 (page 166)) this runs in $O(n+m)$ time.

Other notions of connectivity also arise in practice:

- *What if my graph is directed?* – There are two distinct notions of connected components for directed graphs. A directed graph is *weakly connected* if it would be connected by ignoring the direction of edges. Thus, a weakly connected graph consists of a single piece. A directed graph is *strongly connected* if there is a directed path between every pair of vertices. This distinction is best made clear by considering the network of one- and two-way streets in any city. The network is strongly connected if it is possible to drive legally between every two positions. The network is weakly connected when it is possible to drive legally or *illegally* between every two positions. The network is disconnected if there is no possible way to drive from a to b.

  Weakly and strongly connected components define unique partitions of the vertices. The output figure at the beginning of this section illustrates a directed graph consisting of two weakly or five strongly-connected components (also called *blocks* of G).

  Testing whether a directed graph is weakly connected can be done easily in linear time. Simply turn all edges of G into undirected edges and use the DFS-based connected components algorithm described previously. Tests for strong connectivity are somewhat more complicated. The simplest linear-time algorithm performs a search from some vertex v to demonstrate that the entire graph is reachable from v. We then construct a graph G' where we reverse all the edges of G. A traversal of G' from v suffices to decide whether all vertices of G can reach v. Graph G is strongly connected iff all vertices can reach, and are reachable, from v.

  All the strongly connected components of G can be extracted in linear time using more sophisticated DFS-based algorithms. A generalization of the above "two-DFS" idea is deceptively easy to program but somewhat subtle to understand exactly why it works:

  1. Perform a DFS, starting from an arbitrary vertex in G, and labeling each vertex in order of its completion (not discovery).
  2. Reverse the direction of each edge in G, yielding G'.
  3. Perform a DFS of G', starting from the highest numbered vertex in G. If this search does not completely traverse G', continue with the highest numbered unvisited vertex.
  4. Each DFS tree created in Step 3 is a strongly connected component.

My implementation of a single-pass algorithm appears in Section 5.10.2 (page 181). In either case, it is probably easier to start from an existing implementation than a textbook description.

- *What is the weakest point in my graph/network?* – A chain is only as strong as its weakest link. Losing one or more internal links causes a chain to become disconnected. The *connectivity* of graphs measures their strength—how many edges or vertices must be removed to disconnect it. Connectivity is an essential invariant for network design and other structural problems.

  Algorithmic connectivity problems are discussed in Section 15.8 (page 505). In particular, *biconnected components* are pieces of the graph that result from cutting the edges incident on a single vertex. All biconnected components can be found in linear time using DFS. See Section 5.9.2 (page 173) for an implementation of this algorithm. Vertices whose deletion disconnects the graph belong to more than one biconnected component, whose edges are uniquely partitioned by components.

- *Is the graph a tree? How can I find a cycle if one exists?* – The problem of cycle identification often arises, particularly with respect to directed graphs. For example, testing if a sequence of conditions can deadlock often reduces to cycle detection. If I am waiting for Fred, and Fred is waiting for Mary, and Mary is waiting for me, there is a cycle and we are all deadlocked.

  For undirected graphs, the analogous problem is tree identification. A tree is, by definition, an undirected, connected graph without any cycles. As described above, a depth-first search can be used to test whether it is connected. If the graph is connected and has $n - 1$ edges for n vertices, it is a tree.

  Depth-first search can be used to find cycles in both directed and undirected graphs. Whenever we encounter a back edge in our DFS—i.e. , an edge to an ancestor vertex in the DFS tree—the back edge and the tree together define a directed cycle. No other such cycle can exist in a directed graph. Directed graphs without cycles are called DAGs (directed acyclic graphs). Topological sorting (see Section 15.2 (page 481)) is the fundamental operation on DAGs.

Implementations: The graph data structure implementations of Section 12.4 (page 381) all include implementations of BFS/DFS, and hence connectivity testing to at least some degree. The C++ Boost Graph Library [SLL02] (*http://www.boost.org/libs/graph/doc*) provides implementations of connected components and strongly connected components. LEDA (see Section 19.1.1 (page 658)) provides these plus biconnected and triconnected components, breadth-first and depth-first search, connected components and strongly connected components, all in C++.

With respect to Java, *JUNG* (*http://jung.sourceforge.net/*) also provides biconnected component algorithms, while JGraphT (*http://jgrapht.sourceforge.net/*) does strongly connected components.

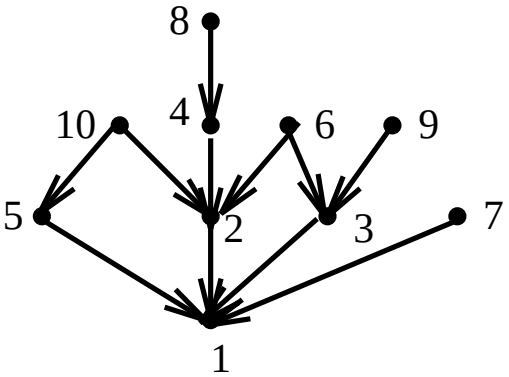
My (biased) preference for C language implementations of all basic graph connectivity algorithms. including strongly connected components and biconnected components, is the library associated with this book. See Section 19.1.10 (page 661) for details.

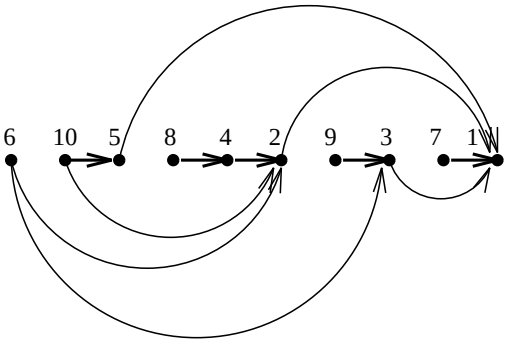
Notes: Depth-first search was first used to find paths out of mazes, and dates back to the nineteenth century [Luc91, Tar95]. Breadth-first search was first reported to find the shortest path by Moore in 1957 [Moo59].

Hopcroft and Tarjan [HT73b, Tar72] established depth-first search as a fundamental technique for efficient graph algorithms. Expositions on depth-first and breadth-first search appear in every book discussing graph algorithms, with [CLRS01] perhaps the most thorough description available.

The first linear-time algorithm for strongly connected components is due to Tarjan [Tar72], with expositions including [BvG99, Eve79a, Man89]. Another algorithm—simpler to program and slicker—for finding strongly connected components is due to Sharir and Kosaraju. Good expositions of this algorithm appear in [AHU83, CLRS01]. Cheriyan and Mehlhorn [CM96] propose improved algorithms for certain problems on dense graphs, including strongly connected components.

Related Problems: Edge-vertex connectivity (see page 505), shortest path (see page 489).





INPUT OUTPUT

15.2 Topological Sorting

Input description: A directed acyclic graph $G = (V, E)$, also known as a *partial order* or *poset*.

Problem description: Find a linear ordering of the vertices of V such that for each edge $(i, j) \in E$, vertex i is to the left of vertex j.

Discussion: Topological sorting arises as a subproblem in most algorithms on directed acyclic graphs. Topological sorting orders the vertices and edges of a DAG in a simple and consistent way and hence plays the same role for DAGs that a depth-first search does for general graphs.

Topological sorting can be used to schedule tasks under precedence constraints. Suppose we have a set of tasks to do, but certain tasks have to be performed before other tasks. These precedence constraints form a directed acyclic graph, and any topological sort (also known as a *linear extension*) defines an order to do these tasks such that each is performed only after all of its constraints are satisfied.

Three important facts about topological sorting are

1. *Only* DAGs can be topologically sorted, since any directed cycle provides an inherent contradiction to a linear order of tasks.

2. *Every* DAG can be topologically sorted, so there must always be at least one schedule for any reasonable precedence constraints among jobs.

3. DAGs can often be topologically sorted in many different ways, especially when there are few constraints. Consider n unconstrained jobs. Any of the $n!$ permutations of the jobs constitutes a valid topological ordering.

The conceptually simplest linear-time algorithm for topological sorting performs a depth-first search of the DAG to identify the complete set of *source vertices*, where source vertices are vertices of in-degree zero. At least one such source must exist in any DAG. Source vertices can appear at the start of any schedule without violating any constraints. Deleting all the outgoing edges of these source vertices will create new source vertices, which can then sit comfortably to the immediate right of the first set. We repeat until all vertices are accounted for. A modest amount of care with data structures (adjacency lists and queues) is sufficient to make this run in $O(n + m)$ time.

An alternate algorithm makes use of the observation that ordering the vertices in terms of decreasing DFS finishing time yields a linear extension. An implementation of this algorithm with an argument for correctness is given in Section 5.10.1 (page 179).

Two special considerations with respect to topological sorting are:

- *What if I need all the linear extensions, instead of just one of them?* – In certain applications, it is important to construct *all* linear extensions of a DAG. Beware, because the number of linear extensions can grow exponentially in the size of the graph. Even the problem of counting the number of linear extensions is NP-hard.

  Algorithms for listing all linear extensions in a DAG are based on backtracking. They build all possible orderings from left to right, where each of the in-degree zero vertices are candidates for the next vertex. The outgoing edges from the selected vertex are deleted before moving on. An optimal algorithm for listing (or counting) linear extensions is discussed in the notes.

  Algorithms for constructing random linear extensions start from an arbitrary linear extension. We then repeatedly sample pairs of vertices. These are exchanged if the resulting permutation remains a topological ordering. This results in a random linear extension given enough random samples. See the Notes section for details.

- *What if your graph is not acyclic?* – When a set of constraints contains inherent contradictions, the natural problem becomes removing the smallest set of items that eliminates all inconsistencies. The sets of offending jobs (vertices) or constraints (edges) whose deletion leaves a DAG are known as the *feedback vertex set* and the *feedback arc set*, respectively. They are discussed in Section 16.11 (page 559). Unfortunately, both problems are NP-complete.

  Since the topological sorting algorithm gets stuck as soon as it identifies a vertex on a directed cycle, we can delete the offending edge or vertex and continue. This quick-and-dirty heuristic will eventually leave a DAG, but might delete more things than necessary. Section 9.10.3 (page 348) describes a better approach to the problem.

Implementations: Essentially all the graph data structure implementations of Section 12.4 (page 381) include implementations of topological sorting. This means the Boost Graph Library [SLL02] (*http://www.boost.org/libs/graph/doc*) and LEDA (see Section 19.1.1 (page 658)) for C++. For Java, the *Data Structures Library in Java* (JDSL) (*http://www.jdsl.org/*) includes a special routine to compute a unit-weighted topological numbering. Also check out JGraphT (*http://jgrapht.sourceforge.net/*).

The *Combinatorial Object Server* (*http://theory.cs.uvic.ca/*) provides C language programs to generate linear extensions in both lexicographic and Gray code orders, as well as count them. An interactive interface is also provided.

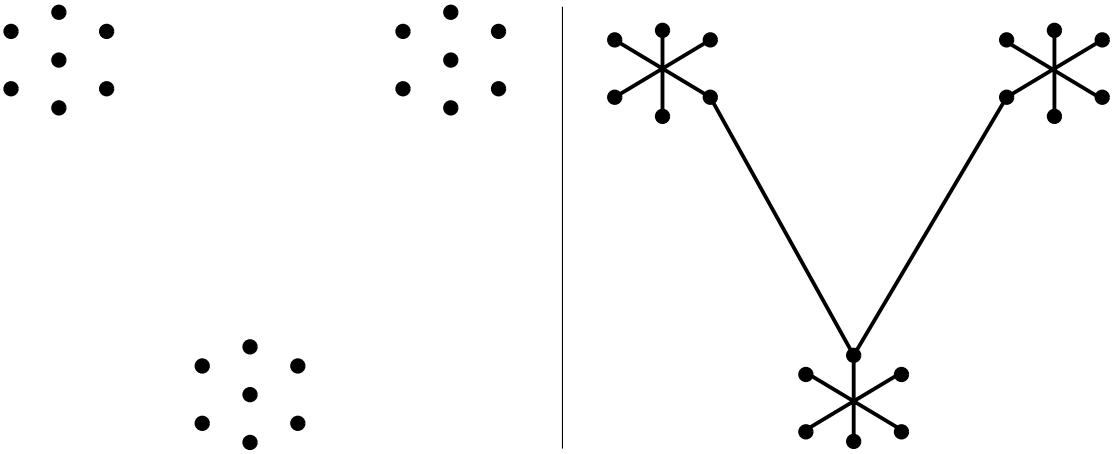
My (biased) preference for C language implementations of all basic graph algorithms, including topological sorting, is the library associated with this book. See Section 19.1.10 (page 661) for details.

Notes: Good expositions on topological sorting include [CLRS01, Man89]. Brightwell and Winkler [BW91] prove that it is #P-complete to count the number of linear extensions of a partial order. The complexity class #P includes NP, so any #P-complete problem is at least NP-hard.

Pruesse and Ruskey [PR86] give an algorithm that generates linear extensions of a DAG in constant amortized time. Further, each extension differs from its predecessor by either one or two adjacent transpositions. This algorithm can be used to count the number of linear extensions $e(G)$ of an n-vertex DAG G in $O(n^2 + e(G))$. Alternately, the reverse search technique of Avis and Fukuda [AF96] can be employed to list linear extensions. A backtracking program to generate all linear extensions is described in [KS74].

Huber [Hub06] gives an algorithm to sample linear extensions uniformly at random from an arbitrary partial order in expected $O(n^3 \lg n)$ time, improving the result of [BD99].

Related Problems: Sorting (see page 436), feedback edge/vertex set (see page 559).



INPUT OUTPUT

15.3 Minimum Spanning Tree

Input description: A graph $G = (V, E)$ with weighted edges.

Problem description: The minimum weight subset of edges $E' \subset E$ that form a tree on V.

Discussion: The minimum spanning tree (MST) of a graph defines the cheapest subset of edges that keeps the graph in one connected component. Telephone companies are interested in minimum spanning trees, because the MST of a set of locations defines the wiring scheme that connects the sites using as little wire as possible. MST is the mother of all network design problems.

Minimum spanning trees prove important for several reasons:

- They can be computed quickly and easily, and create a sparse subgraph that reflects a lot about the original graph.
- They provide a way to identify clusters in sets of points. Deleting the long edges from an MST leaves connected components that define natural clusters in the data set, as shown in the output figure above.
- They can be used to give approximate solutions to hard problems such as Steiner tree and traveling salesman.
- As an educational tool, MST algorithms provide graphic evidence that greedy algorithms can give provably optimal solutions.

Three classical algorithms efficiently construct MSTs. Detailed implementations of two of them (Prim's and Kruskal's) are given with correctness arguments in Section 6.1 (page 192). The third somehow manages to be less well known despite being invented first and (arguably) being both easier to implement and more efficient.

The contenders are

- *Kruskal's algorithm* – Each vertex starts as a separate tree and these trees merges together by repeatedly adding the lowest cost edge that spans two distinct subtrees (i.e. , does not create a cycle).

```
Kruskal(G)
    Sort the edges in order of increasing weight
    count = 0
    while (count < n − 1) do
        get next edge (v, w)
        if (component (v) ≠ component(w))
            add to T
            component(v) = component(w)
```

  The "which component?" tests can be efficiently implemented using the union-find data structure (Section 12.5 (page 385)) to yield an $O(m \lg m)$ algorithm.

- *Prim's algorithm* – Starts with an arbitrary vertex v and "grows" a tree from it, repeatedly finding the lowest-cost edge that links some new vertex into this tree. During execution, we label each vertex as either in the tree, in the *fringe* (meaning there exists an edge from a tree vertex), or *unseen* (meaning the vertex is still more than one edge away from the tree).

```
Prim(G)
    Select an arbitrary vertex to start
    While (there are fringe vertices)
        select minimum-weight edge between tree and fringe
        add the selected edge and vertex to the tree
        update the cost to all affected fringe vertices
```

  This creates a spanning tree for any connected graph, since no cycle can be introduced via edges between tree and fringe vertices. That it is in fact a tree of minimum weight can be proven by contradiction. With simple data structures, Prim's algorithm can be implemented in $O(n^2)$ time.

- *Boruvka's algorithm* – Rests on the observation that the lowest-weight edge incident on each vertex must be in the minimum spanning tree. The union of these edges will result in a spanning forest of at most $n/2$ trees. Now for each of these trees T, select the edge (x, y) of lowest weight such that $x \in T$ and

$y \notin T$. Each of these edges must again be in an MST, and the union again results in a spanning forest with at most half as many trees as before:

```
Boruvka(G)
    Initialize spanning forest F to n single-vertex trees
        While (F has more than one tree)
            for each T in F, find the smallest edge from T to G − T
            add all selected edges to F, thus merging pairs of trees
```

The number of trees are at least halved in each round, so we get the MST after at most $\lg n$ iterations, each of which takes linear time. This gives an $O(m \log n)$ algorithm without using any fancy data structures.

MST is only one of several spanning tree problems that arise in practice. The following questions will help you sort your way through them:

- *Are the weights of all edges of your graph identical?* – Every spanning tree on n points contains exactly $n-1$ edges. Thus, if your graph is unweighted, *any* spanning tree will be a minimum spanning tree. Either breadth-first or depth-first search can be used to find a rooted spanning tree in linear time. DFS trees tend to be long and thin, while BFS trees better reflect the distance structure of the graph, as discussed in Section 5 (page 145).

- *Should I use Prim's or Kruskal's algorithm?* – As implemented in Section 6.1 (page 192), Prim's algorithm runs in $O(n^2)$, while Kruskal's algorithm takes $O(m \log m)$ time. Thus Prim's algorithm is faster on dense graphs, while Kruskal's is faster on sparse graphs.

  That said, Prim's algorithm can be implemented in $O(m + n \lg n)$ time using more advanced data structures, and a Prim's implementation using pairing heaps would be the fastest practical choice for both sparse and dense graphs.

- *What if my input is points in the plane, instead of a graph?* – Geometric instances, comprising n points in d-dimensions, can be solved by constructing the complete distance graph in $O(n^2)$ and then finding the MST of this complete graph. However, for points in two dimensions, it is more efficient to solve the geometric version of the problem directly. To find the minimum spanning tree of n points, first construct the Delaunay triangulation of these points (see Sections 17.3 and 17.4). In two dimensions, this gives a graph with $O(n)$ edges that contains all the edges of the minimum spanning tree of the point set. Running Kruskal's algorithm on this sparse graph finishes the job in $O(n \lg n)$ time.

- *How do I find a spanning tree that avoids vertices of high degree?* – Another common goal of spanning tree problems is to minimize the maximum degree,

typically to minimize the fan out in an interconnection network. Unfortunately, finding a spanning tree of maximum degree 2 is NP-complete, since this is identical to the Hamiltonian path problem. However, efficient algorithms are known that construct spanning trees whose maximum degree is at most one more than required. This is likely to suffice in practice. See the references below.

Implementations: All the graph data structure implementations of Section 12.4 (page 381) *should* include implementations of Prim's and/or Kruskal's algorithms. This includes the Boost Graph Library [SLL02] (*http://www.boost.org/libs/graph/doc*) and LEDA (see Section 19.1.1 (page 658)) for C++. For some reason it does not seem to include the Java graph libraries oriented around social networks, but Prim and Kruskal are present in the *Data Structures Library in Java* (JDSL) (*http://www.jdsl.org/*).

Timing experiments on MST algorithms produce contradicting results, suggesting the stakes are really too low to matter. Pascal implementations of Prim's, Kruskal's, and the Cheriton-Tarjan algorithm are provided in [MS91], along with extensive empirical analysis proving that Prim's algorithm with the appropriate priority queue is fastest on most graphs. The programs in [MS91] are available by anonymous FTP from *cs.unm.edu* in directory */pub/moret_shapiro*. Kruskal's algorithm proved the fastest of four different MST algorithms in the Stanford GraphBase (see Section 19.1.8 (page 660)).

Combinatorica [PS03] provides Mathematica implementations of Kruskal's MST algorithm and quickly counting the number of spanning trees of a graph. See Section 19.1.9 (page 661).

My (biased) preference for C language implementations of all basic graph algorithms, including minimum spanning trees, is the library associated with this book. See Section 19.1.10 (page 661) for details.

Notes: The MST problem dates back to Boruvka's algorithm in 1926. Prim's [Pri57] and Kruskal's [Kru56] algorithms did not appear until the mid-1950's. Prim's algorithm was then rediscovered by Dijkstra [Dij59]. See [GH85] for more on the interesting history of MST algorithms. Wu and Chao [WC04b] have written a monograph on MSTs and related problems.

The fastest implementations of Prim's and Kruskal's algorithms use Fibonacci heaps [FT87]. However, pairing heaps have been proposed to realize the same bounds with less overhead. Experiments with pairing heaps are reported in [SV87].

A simple combination of Boruvka's algorithm with Prim's algorithm yields an $O(m \lg \lg n)$ algorithm. Run Borukva's algorithm for $\lg \lg n$ iterations, yielding a forest of at most $n/\lg n$ trees. Now create a graph G' with one vertex for each tree in this forest, with the weight of the edge between trees T_i and T_j set to the lightest edge (x, y), where $x \in T_i$ and $y \in T_j$. The MST of G' coupled with the edges selected by Boruvka's algorithm yields the MST of G. Prim's algorithm (implemented with Fibonacci heaps) will take $O(n + m)$ time on this $n/\lg n$ vertex, m edge graph.

The best theoretical bounds on finding MSTs tell a complicated story. Karger, Klein, and Tarjan [KKT95] give a linear-time randomized algorithm for MSTs, based again on Borukva's algorithm. Chazelle [Cha00] gave a deterministic $O(n\alpha(m,n))$ algorithm, where $\alpha(m,n)$ is the inverse Ackerman function. Pettie and Ramachandran [PR02] give an provably optimal algorithm whose exact running time is (paradoxically) unknown, but lies between $\Omega(n+m)$ and $O(n\alpha(m,n))$.

A *spanner* $S(G)$ of a given graph G is a subgraph that offers an effective compromise between two competing network objectives. To be precise, they have total weight close to the MST of G, while guaranteeing that the shortest path between vertices x and y in $S(G)$ approaches the shortest path in the full graph G. The monograph of Narasimhan and Smid [NS07] provides a complete, up-to-date survey on spanner networks.

The $O(n \log n)$ algorithm for Euclidean MSTs is due to Shamos, and discussed in computational geometry texts such as [dBvKOS00, PS85].

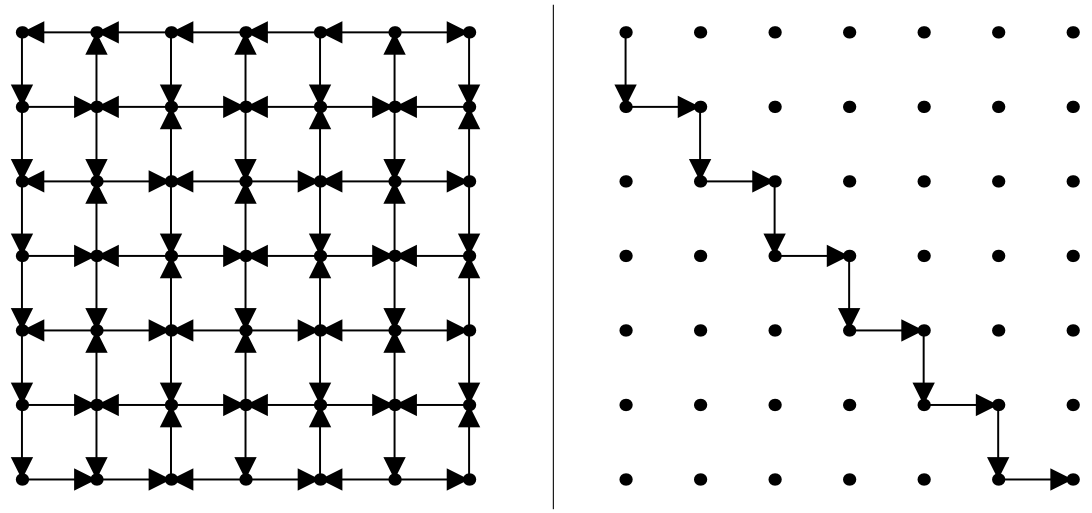
Fürer and Raghavachari [FR94] give an algorithm that constructs a spanning tree whose maximum degree is almost minimized—indeed is at most one more than the lowest-degree spanning tree. The situation is analogous to Vizing's theorem for edge coloring, which also gives an approximation algorithm to within additive factor one. A recent generalization [SL07] gives a polynomial-time algorithm for finding a spanning tree of maximum degree $\leq k+1$ whose cost is no more than that of the optimal minimum spanning tree of maximum degree $\leq k$.

Minimum spanning tree algorithms have an interpretation in terms of *matroids*, which are systems of subsets closed under inclusion. The maximum weighted independent set in matroids can be found using a greedy algorithm. The connection between greedy algorithms and matroids was established by Edmonds [Edm71]. Expositions on the theory of matroids include [Law76, PS98].

Dynamic graph algorithms seek to maintain an graph invariant (such as the MST) efficiently under edge insertion or deletion operations. Holm et al. [HdlT01] gives an efficient, deterministic algorithm to maintain MSTs (and several other invariants) in amortized polylogarithmic time per update.

Algorithms for generating spanning trees in order from minimum to maximum weight are presented in [Gab77]. The complete set of spanning trees of an unweighted graph can be generated in constant amortized time. See Ruskey [Rus03] for an overview of algorithms for generating, ranking, and unranking spanning trees.

Related Problems: Steiner tree (see page 555), traveling salesman (see page 533).



INPUT OUTPUT

15.4 Shortest Path

Input description: An edge-weighted graph G, with vertices s and t.

Problem description: Find the shortest path from s to t in G.

Discussion: The problem of finding shortest paths in a graph has several applications, some quite surprising:

- The most obvious applications arise in transportation or communications, such as finding the best route to drive between Chicago and Phoenix or figuring how to direct packets to a destination across a network.
- Consider the task of partitioning a digitized image into regions containing distinct objects—a problem known as *image segmentation*. Separating lines are needed to carve the space into regions, but what path should these lines take through the grid? We may want a line that relatively directly goes from x to y, but avoids cutting through object pixels as much as possible. This grid of pixels can be modeled as a graph, with the cost of an edge reflecting the color transitions between neighboring pixels. The shortest path from x to y in this weighted graph defines the best separating line.
- *Homophones* are words that sound alike, such as *to*, *two*, and *too*. Distinguishing between homophones is a major problem in speech recognition systems.

The key is to bring some notion of grammatical constraints into the interpretation. We map each string of phonemes (recognized sounds) into words they might possibly match. We construct a graph whose vertices correspond to these possible word interpretations, with edges between neighboring word-interpretations. If we set the weight of each edge to reflect the likelihood of transition, the shortest path across this graph defines the best interpretation of the sentence. See Section 6.4 (page 212) for a more detailed account of a similar application.

- Suppose we want to draw an informative visualization of a graph. The "center" of the graph should appear near the center of the page. A good definition of the graph center is the vertex that minimizes the maximum distance to any other vertex in the graph. Identifying this center point requires knowing the distance (i.e. , shortest path) between all pairs of vertices.

The primary algorithm for finding shortest paths is *Dijkstra's algorithm*, which efficiently computes the shortest path from a given starting vertex x to all $n-1$ other vertices. In each iteration, it identifies a new vertex v for which the shortest path from x to v is known. We maintain a set of vertices S to which we currently know the shortest path from v, and this set grows by one vertex in each iteration. In each iteration, we identify the edge (u, v) where $u, u' \in S$ and $v, v' \in V - S$ such that

$$dist(x, u) + weight(u, v) = \min_{(u', v') \in E} dist(x, u') + weight(u', v')$$

This edge (u, v) gets added to a *shortest path tree*, whose root is x and describes all the shortest paths from x.

An $O(n^2)$ implementation of Dijkstra's algorithm appears in in Section 6.3.1 (page 206). Theoretically faster times can be achieved using significantly more complicated data structures, as described below. If we just need to know the shortest path from x to y, terminate the algorithm as soon as y enters S.

Dijkstra's algorithm is the right choice for single-source shortest path on positively weighted graphs. However, special circumstances dictate different choices:

- *Is your graph weighted or unweighted?* – If your graph is unweighted, a simple breadth-first search starting from the source vertex will find the shortest path to all other vertices in linear time. Only when edges have different weights do you need more sophisticated algorithms. A breadth-first search is both simpler and faster than Dijkstra's algorithm.

- *Does your graph have negative cost weights?* – Dijkstra's algorithm assumes that all edges have positive cost. For graphs with edges of negative weight, you must use the more general, but less efficient, Bellman-Ford algorithm. Graphs with negative cost cycles are an even bigger problem. Observe that the shortest x to y path in such a graph is not defined because we can detour

from x to the negative cost cycle and repeatedly loop around it, making the total cost arbitrarily small.

Note that adding a fixed amount of weight to make each edge positive *does not* solve the problem. Dijkstra's algorithm will then favor paths using a fewer number of edges, even if those were not the shortest weighted paths in the original graph.

- *Is your input a set of geometric obstacles instead of a graph?* – Many applications seek the shortest path between two points in a geometric setting, such as an obstacle-filled room. The most straightforward solution is to convert your problem into a graph of distances to feed to Dijkstra's algorithm. Vertices will correspond the vertices on the boundaries of the obstacles, with edges defined only between pairs of vertices that "see" each other.

  Alternately, there are more efficient geometric algorithms that compute the shortest path directly from the arrangement of obstacles. See Section 17.14 (page 610) on motion planning and the Notes section for pointers to such geometric algorithms.

- *Is your graph acyclic—i.e. , a DAG?* – Shortest paths in directed acyclic graphs can be found in linear time. Perform a topological sort to order the vertices such that all edges go from left to right starting from source s. The distance from s to itself, $d(s, s)$, clearly equals 0. We now process the vertices from left to right. Observe that

$$d(s, j) = \min_{(x,i) \in E} d(s, i) + w(i, j)$$

  since we already know the shortest path $d(s, i)$ for all vertices to the left of j. Indeed, most dynamic programming problems can be formulated as shortest paths on specific DAGs. Note that the same algorithm (replacing min with max) also suffices to find the *longest path* in a DAG, which is useful in many applications like scheduling (see Section 14.9 (page 468)).

- *Do you need the shortest path between all pairs of points?* – If you are interested in the shortest path between all pairs of vertices, one solution is to run Dijkstra n times, once with each vertex as the source. The Floyd-Warshall algorithm is a slick $O(n^3)$ dynamic programming algorithm for all-pairs shortest path, which is faster and easier to program than Dijkstra. It works with negative cost edges but not cycles, and is presented with an implementation in Section 6.3.2 (page 210). Let M denote the distance matrix, where $M_{ij} = \infty$ if there is no edge (i, j):

$$D^0 = M$$
$$\text{for } k = 1 \text{ to } n \text{ do}$$
$$\quad \text{for } i = 1 \text{ to } n \text{ do}$$

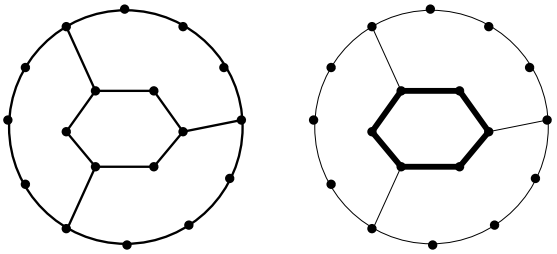


Figure 15.1: The girth, or shortest cycle, in a graph

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for $j = 1$ to n do
$D_{ij}^k = \min(D_{ij}^{k-1}, D_{ik}^{k-1} + D_{kj}^{k-1})$
Return D^n

The key to understanding Floyd's algorithm is that D_{ij}^k denotes "the length of the shortest path from i to j that goes through vertices $1, \ldots, k$ as possible intermediate vertices." Note that $O(n^2)$ space suffices, since we only must keep D^k and D^{k-1} around at time k.

- *How do I find the shortest cycle in a graph?* – One application of all-pairs shortest path is to find the shortest cycle in a graph, called its *girth*. Floyd's algorithm can be used to compute d_{ii} for $1 \leq i \leq n$, which is the length of the shortest way to get from vertex i to i—in other words, the shortest cycle through i.

  This *might* be what you want. The shortest cycle through x is likely to go from x to y back to x, using the same edge twice. A *simple* cycle is one that visits no edge or vertex twice. To find the shortest simple cycle, the easiest approach is to compute the lengths of the shortest paths from i to all other vertices, and then explicitly check whether there is an acceptable edge from each vertex back to i.

  Finding the *longest* cycle in a graph includes Hamiltonian cycle as a special case (see Section 16.5), so it is NP-complete.

The all-pairs shortest path matrix can be used to compute several useful invariants related to the center of graph G. The *eccentricity* of vertex v in a graph is the shortest-path distance to the farthest vertex from v. From the eccentricity come other graph invariants. The *radius* of a graph is the smallest eccentricity of any vertex, while the *center* is the set of vertices whose eccentricity is the radius. The *diameter* of a graph is the maximum eccentricity of any vertex.

Implementations: The highest performance shortest path codes are due to Andrew Goldberg and his collaborators, at *http://www.avglab.com/andrew/soft.html*.

In particular, MLB is a C++ short path implementation for non-negative, integer-weighted edges. See [Gol01] for details of the algorithm and its implementation. Its running time is typically only 4-5 times that of a breadth-first search, and it is capable of handling graphs with millions of vertices. High-performance C implementations of both Dijkstra and Bellman-Ford are also available [CGR99].

All the C++ and Java graph libraries discussed in Section 12.4 (page 381) include at least an implementation of Dijkstra's algorithm. The C++ Boost Graph Library [SLL02] (*http://www.boost.org/libs/graph/doc*) has a particularly broad collection, including Bellman-Ford and Johnson's all-pairs shortest-path algorithm. LEDA (see Section 19.1.1 (page 658)) provides good implementations in C++ for all of the shortest-path algorithms we have discussed, including Dijkstra, Bellman-Ford, and Floyd's algorithms. JGraphT (*http://jgrapht.sourceforge.net/*) provides both Dijkstra and Bellman-Ford in Java. C language implementations of Dijkstra and Floyd's algorithms are provided in the library from this book. See Section 19.1.10 (page 661) for details.

Shortest-path algorithms was the subject of the 9th DIMACS Implementation Challenge, held in October 2006. Implementations of efficient algorithms for several aspects of finding shortest paths were discussed. The papers, instances, and implementations are available at *http://dimacs.rutgers.edu/Challenges/*.

Notes: Good expositions on Dijkstra's algorithm [Dij59], the Bellman-Ford algorithm [Bel58, FF62], and Floyd's all-pairs-shortest-path algorithm [Flo62] include [CLRS01]. Zwick [Zwi01] provides an up-to-date survey on shortest path algorithms. Geometric shortest-path algorithms are surveyed by Mitchell [PN04].

The fastest algorithm known for single-source shortest-path for positive edge weight graphs is Dijkstra's algorithm with Fibonacci heaps, running in $O(m + n \log n)$ time [FT87]. Experimental studies of shortest-path algorithms include [DF79, DGKK79]. However, these experiments were done before Fibonacci heaps were developed. See [CGR99] for a more recent study. Heuristics can be used to enhance the performance of Dijkstra's algorithm in practice. Holzer, et al. [HSWW05] provide a careful experimental study of how four such heuristics interact together.

Online services like Mapquest quickly find at least an approximate shortest path between two points in enormous road networks. This problem differs somewhat from the shortest-path problems here in that (1) preprocessing costs can be amortized over many point-to-point queries, (2) the backbone of high-speed, long-distance highways can reduce the path problem to identifying the best place to get on and off this backbone, and (3) approximate or heuristic solutions suffice in practice.

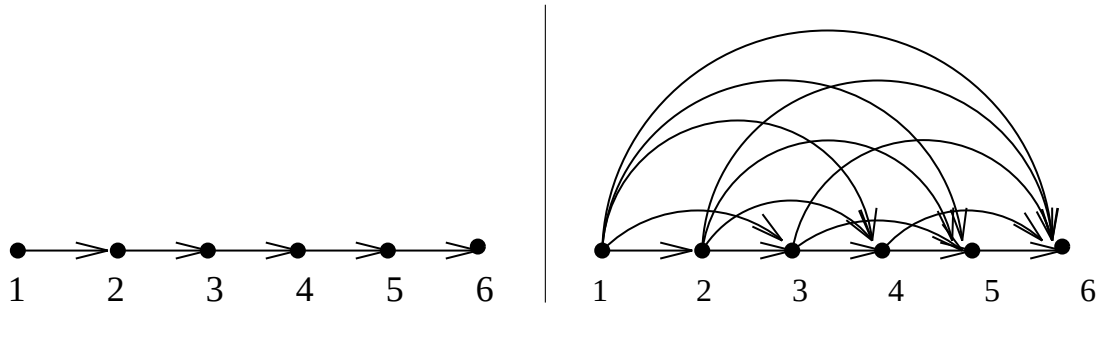
The A^*-algorithm performs a best-first search for the shortest path coupled with a lower-bound analysis to establish when the best path we have seen is indeed the shortest-path in the graph. Goldberg, Kaplan, and Werneck [GKW06, GKW07] describe an implementation of A^* capable of answering point-to-point queries in one millisecond on national-scale road networks after two hours of preprocessing.

Many applications demand multiple alternative short paths in addition to the optimal path. This motivates the problem of finding the k shortest paths. Variants exist depending upon whether the paths must be simple, or can contain cycles. Eppstein [Epp98] generates an implicit representation of these paths in $O(m+n \log n+k)$ time, from which each path

can be reconstructed in $O(n)$ time. Hershberger, et al. [HMS03] present a new algorithm and experimental results.

Fast algorithms for computing the girth are known for both general [IR78] and planar graphs [Dji00].

Related Problems: Network flow (see page 509), motion planning (see page 610).



INPUT OUTPUT

15.5 Transitive Closure and Reduction

Input description: A directed graph $G = (V, E)$.

Problem description: For *transitive closure*, construct a graph $G' = (V, E')$ with edge $(i, j) \in E'$ iff there is a directed path from i to j in G. For *transitive reduction*, construct a small graph $G' = (V, E')$ with a directed path from i to j in G' iff there is a directed path from i to j in G.

Discussion: Transitive closure can be thought of as establishing a data structure that makes it possible to solve reachability questions (can I get to x from y?) efficiently. After constructing the transitive closure, all reachability queries can be answered in constant time by simply reporting the appropriate matrix entry.

Transitive closure is fundamental in propagating the consequences of modified attributes of a graph G. For example, consider the graph underlying any spreadsheet model whose vertices are cells and have an edge from cell i to cell j if the result of cell j depends on cell i. When the value of a given cell is modified, the values of all reachable cells must also be updated. The identity of these cells is revealed by the transitive closure of G. Many database problems reduce to computing transitive closures, for analogous reasons.

There are three basic algorithms for computing transitive closure:

- The simplest algorithm just performs a breadth-first or depth-first search from each vertex and keeps track of all vertices encountered. Doing n such traversals gives an $O(n(n+m))$ algorithm, which degenerates to cubic time if the graph is dense. This algorithm is easily implemented, runs well on sparse graphs, and is likely the right answer for your application.

- Warshall's algorithm constructs transitive closures in $O(n^3)$ using a simple, slick algorithm that is identical to Floyd's all-pairs shortest-path algorithm

of Section 15.4 (page 489). If we are interested only in the transitive closure, and not the length of the resulting paths, we can reduce storage by retaining only one bit for each matrix element. Thus, $D_{ij}^k = 1$ iff j is reachable from i using only vertices $1, \ldots, k$ as intermediates.

- Matrix multiplication can also be used to solve transitive closure. Let M^1 be the adjacency matrix of graph G. The non-zero matrix entries of $M^2 = M \times M$ identify all length-2 paths in G. Observe that $M^2[i,j] = \sum_x M[i,x] \cdot M[x,j]$, so path (i,x,j) contributes to $M^2[i,j]$. Thus, the union $\cup_i^n M^i$ yields the transitive closure T. Furthermore, this union can be computed using only $O(\lg n)$ matrix operations using the fast exponentiation algorithm in Section 13.9 (page 423).

  You might conceivably win for large n by using Strassen's fast matrix multiplication algorithm, although I for one wouldn't bother trying. Since transitive closure is provably as hard as matrix multiplication, there is little hope for a significantly faster algorithm.

The running time of all three of these procedures can be substantially improved on many graphs. Recall that a strongly connected component is a set of vertices for which all pairs are mutually reachable. For example, any cycle defines a strongly connected subgraph. All the vertices in any strongly connected component must reach exactly the same subset of G. Thus, we can reduce our problem finding the transitive closure on a graph of strongly connected components that should have considerably fewer edges and vertices than G. The strongly connected components of G can be computed in linear time (see Section 15.1 (page 477)).

Transitive reduction (also known as *minimum equivalent digraph*) is the inverse operation of transitive closure, namely reducing the number of edges while maintaining identical reachability properties. The transitive closure of G is identical to the transitive closure of the transitive reduction of G. The primary application of transitive reduction is space minimization, by eliminating redundant edges from G that do not effect reachability. Transitive reduction also arises in graph drawing, where it is important to eliminate as many unnecessary edges as possible to reduce the visual clutter.

Although the transitive closure of G is uniquely defined, a graph may have many different transitive reductions, including G itself. We want the smallest such reduction, but there are multiple formulations of the problem:

- A linear-time, quick-and-dirty transitive reduction algorithm identifies the strongly connected components of G, replaces each by a simple directed cycle, and adds these edges to those bridging the different components. Although this reduction is not provably minimal, it is likely to be pretty close on typical graphs.

  One catch with this heuristic is that it might add edges to the transitive reduction of G that are not in G. This may or may not be a problem depending on your application.

- If all edges of our transitive reduction must exist in G, we have to abandon hope of finding the minimum size reduction. To see why, consider a directed graph consisting of one strongly connected component so that every vertex can reach every other vertex. The smallest possible transitive reduction will be a simple directed cycle, consisting of exactly n edges. This is possible if and only if G is Hamiltonian, thus proving that finding the smallest subset of edges is NP-complete.

  A heuristic for finding such a transitive reduction is to consider each edge successively and delete it if its removal does not change the transitive reduction. Implementing this efficiently means minimizing the time spent on reachability tests. Observe that a directed edge (i, j) can be eliminated whenever there is another path from i to j avoiding this edge.

- The minimum size reduction where we are allowed arbitrary pairs of vertices as edges can be found in $O(n^3)$ time. See the references below for details. However, the quick-and-dirty heuristic above will likely suffice for most applications, being easier to program as well as more efficient.

Implementations: The Boost implementation of transitive closure appears particularly well engineered, and relies on algorithms from [Nuu95]. LEDA (see Section 19.1.1 (page 658)) provides implementations of both transitive closure and reduction in C++ [MN99].

None of our usual Java libraries appear to contain implementations of either transitive closure or reduction. However, *Graphlib* contains a Java `Transitivity` library with both of them. See *http://www-verimag.imag.fr/∼cotton/* for details.

Combinatorica [PS03] provides Mathematica implementations of transitive closure and reduction, as well as the display of partial orders requiring transitive reduction. See Section 19.1.9 (page 661).

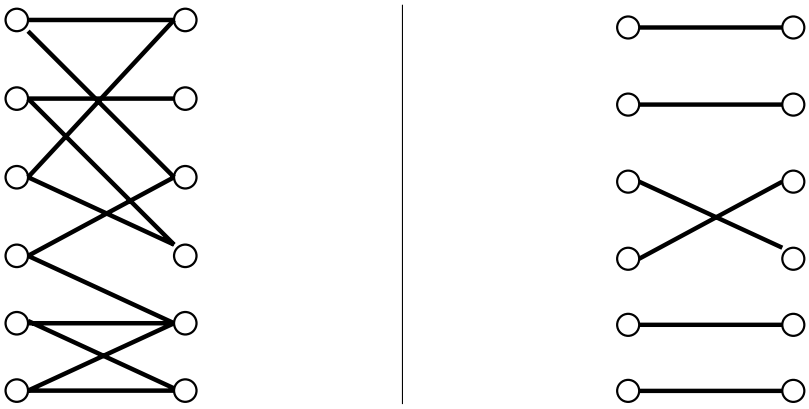
Notes: Van Leeuwen [vL90a] provides an excellent survey on transitive closure and reduction. The equivalence between matrix multiplication and transitive closure was proven by Fischer and Meyer [FM71], with expositions including [AHU74].

There is a surprising amount of recent activity on transitive closure, much of it captured by Nuutila [Nuu95]. Penner and Prasanna [PP06] improved the performance of Warshall's algorithm [War62] by roughly a factor of two through a cache-friendly implementation.

The equivalence between transitive closure and reduction, as well as the $O(n^3)$ reduction algorithm, was established in [AGU72]. Empirical studies of transitive closure algorithms include [Nuu95, PP06, SD75].

Estimating the size of the transitive closure is important in database query optimization. A linear-time algorithm for estimating the size of the closure is given by Cohen [Coh94].

Related Problems: Connected components (see page 477), shortest path (see page 489).



INPUT OUTPUT

15.6 Matching

Input description: A (weighted) graph $G = (V, E)$.

Problem description: Find the largest set of edges E' from E such that each vertex in V is incident to at most one edge of E'.

Discussion: Suppose we manage a group of workers, each of whom is capable of performing a subset of the tasks needed to complete a job. Construct a graph with vertices representing both the set of workers and the set of tasks. Edges link workers to the tasks they can perform. We must assign each task to a different worker so that no worker is overloaded. The desired assignment is the largest possible set of edges where no employee or job is repeated—i.e. , a matching.

Matching is a very powerful piece of algorithmic magic, so powerful that it is surprising that optimal matchings can be found efficiently. Applications arise often once you know to look for them.

Marrying off a set of boys to a set of girls such that each couple is happy is another bipartite matching problem, on a graph with an edge between any compatible boy and girl. For a synthetic biology application [MPC+06], I need to shuffle the characters in a string S to maximize the number of characters that move. For example, *aaabc* can be shuffled to *bcaaa* so that only one character stays fixed. This is yet another bipartite matching problem, where the boys represent the multiset of alphabet symbols and the girls are the positions in the string (1 to $|S|$). Edges link symbols to all the string positions that originally contained a different symbol.

This basic matching framework can be enhanced in several ways, while remaining essentially the same *assignment* problem:

- *Is your graph bipartite?* – Most matching problems involve bipartite graphs, as in the classic assignment problem of jobs to workers. This is fortunate because faster and simpler algorithms exist for bipartite matching.

- *What if certain employees can be given multiple jobs?* – Natural generalizations of the assignment problem include assigning certain employees more than one task to do, or (equivalently) seeking multiple workers for a given job. Here, we do not seek a matching so much as a covering with small "stars." Such desires can be modeled by replicating an employee vertex by as many times as we want her to be matched. Indeed, we employed this trick in the string permutation example above.

- *Is your graph weighted or unweighted?* – Many matching applications are based on unweighted graphs. Perhaps we seek to maximize the total number of tasks performed, where one task is as good as another. Here we seek a maximum *cardinality* matching—ideally a *perfect* matching where every vertex is matched to another in the matching.

  For other applications, however, we need to augment each edge with a weight, perhaps reflecting the suitability of an employee for a given task. The problem now becomes constructing a maximum *weight* matching—i.e. , the set of independent edges of maximum total cost.

Efficient algorithms for constructing matchings work by constructing *augmenting paths* in graphs. Given a (partial) matching M in a graph G, an augmenting path is a path of edges P that alternate (out-of-M, in-M, ..., out-of-M). We can enlarge the matching by one edge given such an augmenting path, replacing the even-numbered edges of P from M with the odd-numbered edges of P. Berge's theorem states that a matching is maximum if and only if it does not contain any augmenting path. Therefore, we can construct maximum-cardinality matchings by searching for augmenting paths and stopping when none exist.

General graphs prove trickier because it is possible to have augmenting paths that are odd-length cycles (i.e. , the first and last vertices are the same). Such cycles (or blossoms) are impossible in bipartite graphs, which by definition do not contain odd-length cycles.

The standard algorithms for bipartite matching are based on network flow, using a simple transformation to convert a bipartite graph into an equivalent flow graph. Indeed, an implementation of this is given in Section 6.5 (page 217).

Be warned that different approaches are needed to solve weighted matching problems, most notably the matrix-oriented "Hungarian algorithm."

Implementations: High-performance codes for both weighted and unweighted bipartite matching have been developed by Andrew Goldberg and his collaborators. `CSA` is a weighted bipartite matching code in C based on cost-scaling network flow, developed by Goldberg and Kennedy [GK95]. `BIM` is a faster unweighted bipartite matching code based on augmenting path methods, developed

by Cherkassky, et al. [CGM+98]. Both are available for noncommercial use from *http://www.avglab.com/andrew/soft.html*.

The First DIMACS Implementation Challenge [JM93] focused on network flows and matching. Several instance generators and implementations for maximum weight and maximum cardinality matching were collected, and can be obtained by anonymous FTP from *dimacs.rutgers.edu* in the directory *pub/netflow/matching*. These include

- A maximum-cardinality matching solver in Fortran 77 by R. Bruce Mattingly and Nathan P. Ritchey.
- A maximum-cardinality matching solver in C by Edward Rothberg, that implements Gabow's $O(n^3)$ algorithm.
- A maximum-weighted matching solver in C by Edward Rothberg. This is slower but more general than his unweighted solver just described.

GOBLIN (*http://www.math.uni-augsburg.de/~fremuth/goblin.html*) is an extensive C++ library dealing with all of the standard graph optimization problems, including weighted bipartite matching. LEDA (see Section 19.1.1 (page 658)) provides efficient implementations in C++ for both maximum-cardinality and maximum-weighted matching, on both bipartite and general graphs.

Blossum IV [CR99] is an efficient code in C for minimum-weight perfect matching available at *http://www2.isye.gatech.edu/~wcook/software.html*. An $O(mn\alpha(m,n))$ implementation of maximum-cardinality matching in general graphs (*http://www.cs.arizona.edu/~kece/Research/software.html*) is due to Kececioglu and Pecqueur [KP98].

The Stanford GraphBase (see Section 19.1.8 (page 660)) contains an implementation of the Hungarian algorithm for bipartite matching. To provide readily visualized weighted bipartite graphs, Knuth uses a digitized version of the Mona Lisa and seeks row/column disjoint pixels of maximum brightness. Matching is also used to construct clever, resampled "domino portraits".

Notes: Lovász and Plummer [LP86] is the definitive reference on matching theory and algorithms. Survey articles on matching algorithms include [Gal86]. Good expositions on network flow algorithms for bipartite matching include [CLRS01, Eve79a, Man89], and those on the Hungarian method include [Law76, PS98]. The best algorithm for maximum bipartite matching, due to Hopcroft and Karp [HK73], repeatedly finds the shortest augmenting paths instead of using network flow, and runs in $O(\sqrt{n}m)$. The Hungarian algorithm runs in $O(n(m + n \log n))$ time.

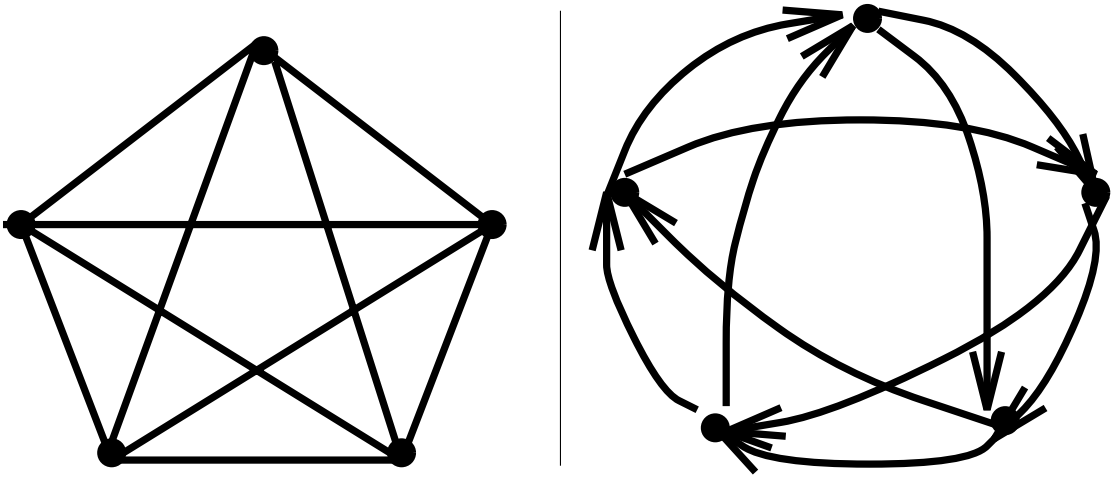
Edmond's algorithm [Edm65] for maximum-cardinality matching is of great historical interest for provoking questions on what problems can be solved in polynomial time. Expositions on Edmond's algorithm include [Law76, PS98, Tar83]. Gabow's [Gab76] implementation of Edmond's algorithm runs in $O(n^3)$ time. The best algorithm known for general matching runs in $O(\sqrt{n}m)$ [MV80].

Consider a matching of boys to girls containing edges (B_1, G_1) and (B_2, G_2), where B_1 and G_2 in fact prefer each other to their own spouses. In real life, these two would

run off with each other, breaking the marriages. A marriage without any such couples is said to be *stable*. The theory of stable matching is thoroughly treated in [GI89]. It is a surprising fact that no matter how the boys and girls rate each other, there is always at least one stable marriage. Further, such a marriage can be found in $O(n^2)$ time [GS62]. An important application of stable marriage occurs in the annual matching of medical residents to hospitals.

The maximum matching is equal in size to the minimum vertex cover in bipartite graphs. This implies that both the minimum vertex cover problem and maximum independent set problems can be solved in polynomial time on bipartite graphs.

Related Problems: Eulerian cycle (see page 502), network flow (see page 509).



INPUT OUTPUT

15.7 Eulerian Cycle/Chinese Postman

Input description: A graph $G = (V, E)$.

Problem description: Find the shortest tour visiting each edge of G at least once.

Discussion: Suppose you are given the map of a city and charged with designing the routes for garbage trucks, snow plows, or postmen. In each of these applications, every road in the city must be completely traversed at least once in order to ensure that all deliveries or pickups are made. For efficiency, you seek to minimize total drive time, or (equivalently) the total distance or number of edges traversed.

Alternately, consider a human-factors validation of telephone menu systems. Each "Press 4 for more information" option is properly interpreted as an edge between two vertices in a graph. Our tester seeks the most efficient way to walk over this graph and visit every link in the system at least once.

Such applications are variants of the *Eulerian cycle* problem, best characterized by the puzzle that asks children to draw a given figure completely without (1) without repeating any edges, or (2) lifting their pencil off the paper. They seek a path or cycle through a graph that visits each edge exactly once.

Well-known conditions exist for determining whether a graph contains an Eulerian cycle or path:

- An *undirected* graph contains an Eulerian *cycle* iff (1) it is connected, and (2) each vertex is of even degree.

- An *undirected* graph contains an Eulerian *path* iff (1) it is connected, and (2) all but two vertices are of even degree. These two vertices will be the start and end points of any path.

- A *directed* graph contains an Eulerian *cycle* iff (1) it is strongly-connected, and (2) each vertex has the same in-degree as out-degree.

- Finally, a *directed* graph contains an Eulerian *path* from x to y iff (1) it is connected, and (2) all other vertices have the same in-degree as out-degree, with x and y being vertices with in-degree one less and one more than their out-degrees, respectively.

This characterization of Eulerian graphs makes it is easy to test whether such a cycle exists: verify that the graph is connected using DFS or BFS, and then count the number of odd-degree vertices. Explicitly constructing the cycle also takes linear time. Use DFS to find an arbitrary cycle in the graph. Delete this cycle and repeat until the entire set of edges has been partitioned into a set of edge-disjoint cycles. Since deleting a cycle reduces each vertex degree by an even number, the remaining graph will continue to satisfy the same Eulerian degree-bound conditions. These cycles will have common vertices (since the graph is connected), and so can be spliced together in a "figure eight" at a shared vertex. By so splicing all the extracted cycles together, we construct a single circuit containing all of the edges.

An Eulerian cycle, if one exists, solves the motivating snowplow problem, since any tour that visits each edge only once must have minimum length. However, it is unlikely that your road network happens to satisfy the Eulerian degree conditions. Instead, we need to solve the more general *Chinese postman problem*, which minimizes the length of a cycle that traverses every edge at least once. This minimum cycle will never visit any edge more than twice, so good tours exist for any road network.

The optimal postman tour can be constructed by adding the appropriate edges to the graph G to make it Eulerian. Specifically, we find the shortest path between each pair of odd-degree vertices in G. Adding a path between two odd-degree vertices in G turns both of them to even-degree, moving G closer to becoming an Eulerian graph. Finding the best set of shortest paths to add to G reduces to identifying a minimum-weight perfect matching in a special graph G'.

For undirected graphs, the vertices of G' correspond the odd-degree vertices of G, with the weight of edge (i, j) defined to be the length of the shortest path from i to j in G. For directed graphs, the vertices of G' correspond to the degree-imbalanced vertices from G, with the bonus that all edges in G' go from out-degree deficient vertices to in-degree deficient ones. Thus, bipartite matching algorithms suffice when G is directed. Once the graph is Eulerian, the actual cycle can be extracted in linear time using the procedure just described.

Implementations: Several graph libraries provide implementations of Eulerian cycles, but Chinese postman implementations are rarer. We recommend the imple-

mentation of directed Chinese postman by Thimbleby [Thi03]. This Java implementation is available at *http://www.cs.swan.ac.uk/~csharold/cpp/index.html*.

GOBLIN (*http://www.math.uni-augsburg.de/~fremuth/goblin.html*) is an extensive C++ library dealing with all of the standard graph optimization problems, including Chinese postman for both directed and undirected graphs. LEDA (see Section 19.1.1 (page 658)) provides all the tools for an efficient implementation: Eulerian cycles, matching, and shortest-paths bipartite and general graphs.

Combinatorica [PS03] provides Mathematica implementations of Eulerian cycles and de Bruijn sequences. See Section 19.1.9 (page 661).

Notes: The history of graph theory began in 1736, when Euler [Eul36] first solved the seven bridges of Königsberg problem. Königsberg (now Kaliningrad) is a city on the banks of the Pregel river. In Euler's day there were seven bridges linking the banks and two islands, which can be modeled as a multigraph with seven edges and four vertices. Euler sought a way to walk over each of the bridges exactly once and return home—i.e. , an Eulerian cycle. Euler proved that such a tour is impossible, since all four of the vertices had odd degrees. The bridges were destroyed in World War II. See [BLW76] for a translation of Euler's original paper and a history of the problem.

Expositions on linear-time algorithms for constructing Eulerian cycles [Ebe88] include [Eve79a, Man89]. Fleury's algorithm [Luc91] is a direct and elegant approach to constructing Eulerian cycles. Start walking from any vertex, and erase any edge that has been traversed. The only criterion in picking the next edge is that we avoid using a bridge (an edge whose deletion disconnects the graph) until no other alternative remains.

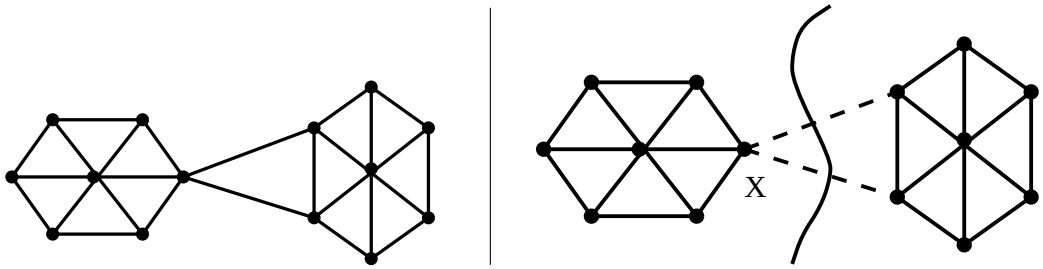
The Euler's tour technique is an important paradigm in parallel graph algorithms. Many parallel graph algorithms start by finding a spanning tree and then rooting the tree, where the rooting is done using the Euler tour technique. See parallel algorithms texts (e.g., [JÓ92]) for an exposition, and [CB04] for recent experience in practice. Efficient algorithms exist to count the number of Eulerian cycles in a graph [HP73].

The problem of finding the shortest tour traversing all edges in a graph was introduced by Kwan [Kwa62], hence the name *Chinese* postman. The bipartite matching algorithm for solving Chinese postman is due to Edmonds and Johnson [EJ73]. This algorithm works for both directed and undirected graphs, although the problem is NP-complete for mixed graphs [Pap76a]. Mixed graphs contain both directed and undirected edges. Expositions of the Chinese postman algorithm include [Law76].

A *de Bruijn* sequence S of span n on an alphabet Σ of size α is a circular string of length α^n containing all strings of length n as substrings of S, each exactly once. For example, for $n = 3$ and $\Sigma = \{0, 1\}$, the circular string 00011101 contains the following substrings in order: 000, 001, 011, 111, 110, 101, 010, 100. De Bruijn sequences can be thought of as "safe cracker" sequences, describing the shortest sequence of dial turns with α positions sufficient to try out all combinations of length n.

De Bruijn sequences can be constructed by building a directed graph whose vertices are all α^{n-1} strings of length $n-1$, where there is an edge (u, v) iff $u = s_1 s_2 \ldots s_{n-1}$ and $v = s_2 \ldots s_{n-1} s_n$. Any Eulerian cycle on this graph describes a de Bruijn sequence. Expositions on de Bruijn sequences and their construction include [Eve79a, PS03].

Related Problems: Matching (see page 498), Hamiltonian cycle (see page 538).



15.8 Edge and Vertex Connectivity

Input description: A graph G. Optionally, a pair of vertices s and t.

Problem description: What is the smallest subset of vertices (or edges) whose deletion will disconnect G? Or which will separate s from t?

Discussion: Graph connectivity often arises in problems related to network reliability. In the context of telephone networks, the vertex connectivity is the smallest number of switching stations that a terrorist must bomb in order to separate the network—i.e. , prevent two unbombed stations from talking to each other. The edge connectivity is the smallest number of wires that need to be cut to accomplish the same objective. One well-placed bomb or snipping the right pair of cables suffices to disconnect the above network.

The edge (vertex) connectivity of a graph G is the smallest number of edge (vertex) deletions sufficient to disconnect G. There is a close relationship between the two quantities. The vertex connectivity is always less than or equal to the edge connectivity, since deleting one vertex from each edge in a cut set succeeds in disconnecting the graph. But smaller vertex subsets may be possible. The minimum vertex degree is an upper bound for both edge and vertex connectivity, since deleting all its neighbors (or cutting the edges to all its neighbors) disconnects the graph into one big and one single-vertex component.

Several connectivity problems prove to be of interest:

- *Is the graph already disconnected?* – The simplest connectivity problem is testing whether the graph is in fact connected. A simple depth-first or breadth-first search suffices to identify all connected components in linear time, as discussed in Section 15.1 (page 477). For directed graphs, the issue is whether the graph is *strongly connected*, meaning there is a directed path between any pair of vertices. In a *weakly connected* graph, there may exist paths to nodes from which there is no way to return.

- *Is there one weak link in my graph?* – We say that G is *biconnected* if no single vertex deletion is sufficient to disconnect G. Any vertex that is such a weak point is called an *articulation vertex*. A *bridge* is the analogous concept for edges, meaning a single edge whose deletion disconnects the graph.

  The simplest algorithms for identifying articulation vertices (or bridges) try deleting vertices (or edges) one by one, and then use DFS or BFS to test whether the resulting graph is still connected. More sophisticated linear-time algorithms exist for both problems, based on depth-first search. Indeed, a full implementation is given in Section 5.9.2 (page 173).

- *What if I want to split the graph into equal-sized pieces?* – What is often sought is a small cut set that breaks the graph into roughly equal-sized pieces. For example, suppose we want to split a big computer program into two maintainable units. We can construct a graph whose the vertices represent subroutines. Edges can be added between any two subroutines that interact, namely where one calls the other. We now seek to partition the subroutines into roughly equal-sized sets so that few pairs of interacting routines span the divide.

  This is the *graph partition* problem, further discussed in Section 16.6 (page 541). Although the problem is NP-complete, reasonable heuristics exist to solve it.

- *Are arbitrary cuts OK, or must I separate a given pair of vertices?* – There are two flavors of the general connectivity problem. One asks for the smallest cut-set for the entire graph, the other for the smallest set to separate s from t. Any algorithm for $(s-t)$ connectivity can be used with each of the $n(n-1)/2$ possible pairs of vertices to give an algorithm for general connectivity. Less obviously, $n-1$ runs suffice for testing edge connectivity, since we know that vertex v_1 must end up in a different component from at least one of the other $n-1$ vertices after deleting any cut set.

Edge and vertex connectivity can both be found using network-flow techniques. Network flow, discussed in Section 15.9 (page 509), interprets a weighted graph as a network of pipes where each edge has a maximum capacity and we seek to maximize the flow between two given vertices of the graph. The maximum flow between v_i, v_j in G is exactly the weight of the smallest set of edges to disconnect v_i from v_j. Thus the edge connectivity can be found by minimizing the flow between v_i and each of the $n-1$ other vertices in an unweighted graph G. Why? After deleting the minimum-edge cut set, v_i will be separated from some other vertex.

Vertex connectivity is characterized by *Menger's theorem*, which states that a graph is k-connected if and only if every pair of vertices is joined by at least k vertex-disjoint paths. Network flow can again be used to perform this calculation, since a flow of k between a pair of vertices implies k *edge*-disjoint paths. To exploit Menger's theorem, we construct a graph G' such that any set of edge-disjoint paths

in G' corresponds to vertex-disjoint paths in G. This is done by replacing each vertex v_i of G with two vertices $v_{i,1}$ and $v_{i,2}$, such that edge $(v_{i,1}, v_{i,2}) \in G'$ for all $v_i \in G$, and by replacing every edge $(v_i, x) \in G$ by edges $(v_{i,j}, x_k)$, $j \neq k \in \{0, 1\}$ in G'. Thus two edge-disjoint paths in G' correspond to each vertex-disjoint path in G.

Implementations: `MINCUTLIB` is a collection of high-performance codes for several different cut algorithms, including both flow and contraction-based methods. They were implemented by Chekuri, et al. as part of a substantial experimental study [CGK+97]. The codes are available for noncommercial use at *http://www.avglab.com/andrew/soft.html*. Also included is the full version of [CGK+97]—an excellent presentation of these algorithms and the heuristics needed to make them run fast.

Most of the graph data structure libraries of Section 15.1 (page 477) include routines for connectivity and biconnectivity testing. The C++ Boost Graph Library [SLL02] (*http://www.boost.org/libs/graph/doc*) is distinguished by also including an implementation of edge connectivity testing.

GOBLIN (*http://www.math.uni-augsburg.de/~fremuth/goblin.html*) is an extensive C++ library dealing with all of the standard graph optimization problems, including both edge and vertex connectivity.

LEDA (see Section 19.1.1 (page 658)) contains extensive support for both low-level connectivity testing (both biconnected and triconnected components) and edge connectivity/minimum-cut in C++.

Combinatorica [PS03] provides Mathematica implementations of edge and vertex connectivity, as well as connected, biconnected, and strongly connected components with bridges and articulation vertices. See Section 19.1.9 (page 661).

Notes: Good expositions on the network-flow approach to edge and vertex connectivity include [Eve79a, PS03]. The correctness of these algorithms is based on Menger's theorem [Men27] that connectivity is determined by the number of edge and vertex disjoint paths separating a pair of vertices. The maximum-flow, minimum-cut theorem is due to Ford and Fulkerson [FF62].

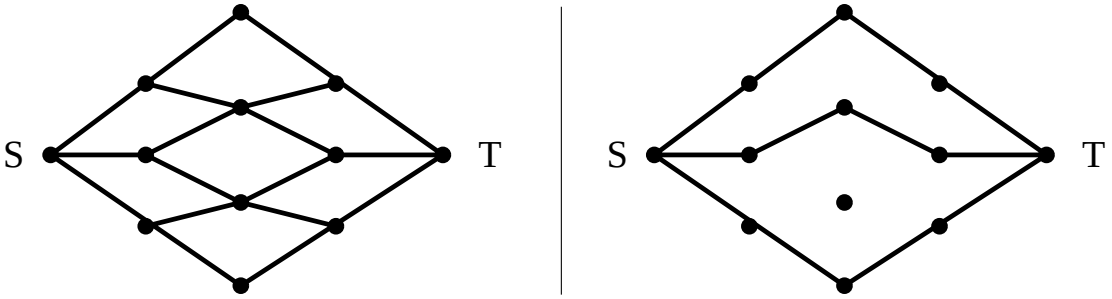
The theoretically fastest algorithms for minimum-cut/edge connectivity are based on graph contraction, not network flows. Contracting an edge (x, y) in a graph G merges the two incident vertices into one, removing self-loops but leaving multiedges. Any sequence of such contractions can raise (but not lower) the minimum cut in G, and leaves the cut unchanged if no edge of the cut is contracted. Karger gave a beautiful randomized algorithm for minimum cut, observing that the minimum cut is left unchanged with nontrivial probability over the course of any random series of deletions. The fastest version of Karger's algorithm runs in $(m \lg^3 n)$ expected time [Kar00]. See Motwani and Raghavan [MR95] for an excellent treatment of randomized algorithms, including a presentation of Karger's algorithm.

Nagamouchi and Ibaraki [NI92] give a deterministic contraction-based algorithm to find the minimum cut in $O(n(m + n \log n))$. In each round, this algorithm identifies and contracts an edge that is provably not in the minimum cut. See [CGK+97, NOI94] for experimental comparisons of algorithms for finding minimum cuts.

Minimum-cut methods have found many applications in computer vision, including image segmentation. Boykov and Kolmogorov [BK04] report on an experimental evaluation of minimum-cut algorithms in this context.

A nonflow-based algorithm for edge k-connectivity in $O(kn^2)$ is due to Matula [Mat87]. Faster k-connectivity algorithms are known for certain small values of k. All three-connected components of a graph can be generated in linear time [HT73a], while $O(n^2)$ suffices to test 4-connectivity [KR91].

Related Problems: Connected components (see page 477), network flow (see page 509), graph partition (see page 541).



INPUT OUTPUT

15.9 Network Flow

Input description: A directed graph G, where each edge $e = (i, j)$ has a capacity c_e. A source node s and sink node t.

Problem description: What is the maximum flow you can route from s to t while respecting the capacity constraint of each edge?

Discussion: Applications of network flow go far beyond plumbing. Finding the most cost-effective way to ship goods between a set of factories and a set of stores defines a network-flow problem, as do many resource-allocation problems in communications networks.

The real power of network flow is (1) that a surprising variety of linear programming problems arising in practice can be modeled as network-flow problems, and (2) that network-flow algorithms can solve these problems much faster than general-purpose linear programming methods. Several graph problems we have discussed in this book can be solved using network flow, including bipartite matching, shortest path, and edge/vertex connectivity.

The key to exploiting this power is recognizing that your problem can be modeled as network flow. This requires experience and study. My recommendation is that you first construct a linear programming model for your problem and then compare it with linear programs for the two primary classes of network flow problems: *maximum flow* and *minimum-cost flow*:

- *Maximum Flow* – Here we seek the heaviest possible flow from s to t, given the edge capacity constraints of G. Let x_{ij} be a variable accounting for the flow from vertex i through directed edge (i, j). The flow through this edge is constrained by its capacity c_{ij}, so

$$0 \leq x_{ij} \leq c_{ij} \text{ for } 1 \leq i, j \leq n$$

Furthermore, an equal flow comes in as goes out at each nonsource or sink vertex, so

$$\sum_{j=1}^{n} x_{ij} - \sum_{j=1}^{n} x_{ji} = 0 \text{ for } 1 \leq i \leq n$$

We seek the assignment that maximizes the flow into sink t, namely $\sum_{i=1}^{n} x_{it}$

- *Minimum Cost Flow* – Here we have an extra parameter for each edge (i, j), namely the cost (d_{ij}) of sending one unit of flow from i to j. We also have a targeted amount of flow f we want to send from s to t at minimum total cost. Hence, we seek the assignment that minimizes

$$\sum_{j=1}^{n} d_{ij} \cdot x_{ij}$$

subject to the edge and vertex capacity constraints of maximum flow, plus the additional restriction that $\sum_{i=1}^{n} x_{it} = f$.

Special considerations include:

- *What if I have multiple sources and/or sinks?* – No problem. We can handle this by modifying the network to create a vertex to serve as a super-source that feeds all the sources, and a super-sink that drains all the sinks.

- *What if all arc capacities are identical, either 0 or 1?* – Faster algorithms exist for 0-1 network flows. See the Notes section for details.

- *What if all my edge costs are identical?* – Use the simpler and faster algorithms for solving maximum flow as opposed to minimum-cost flow. Max-flow without edge costs arises in many applications, including edge/vertex connectivity and bipartite matching.

- *What if I have multiple types of material moving through the network?* – In a telecommunications network, every message has a given source and destination. Each destination needs to receive *exactly* those calls sent to it, not an equal amount of communication from arbitrary places. This can be modeled as a *multicommodity flow* problem, where each call defines a different commodity and we seek to satisfy all demands without exceeding the total capacity of any edge.

  Linear programming will suffice for multicommodity flow if fractional flows are permitted. Unfortunately, integral multicommodity flow is NP-complete, even for only two commodities.

Network flow algorithms can be complicated, and significant engineering is required to optimize performance. Thus, we strongly recommend that you use an existing code rather than implement your own. Excellent codes are available and described below. The two primary classes of algorithms are:

- *Augmenting path methods* – These algorithms repeatedly find a path of positive capacity from source to sink and add it to the flow. It can be shown that the flow through a network is optimal if and only if it contains no augmenting path. Since each augmentation adds something to the flow, we eventually find the maximum. The difference between network-flow algorithms is in *how* they select the augmenting path. If we are not careful, each augmenting path will add but a little to the total flow, and so the algorithm might take a long time to converge.

- *Preflow-push methods* – These algorithms push flows from one vertex to another, initially ignoring the constraint that in-flow must equal out-flow at each vertex. Preflow-push methods prove faster than augmenting-path methods, essentially because multiple paths can be augmented simultaneously. These algorithms are the method of choice and are implemented in the best codes described in the next section.

Implementations: High-performance codes for both maximum flow and minimum cost flow were developed by Andrew Goldberg and his collaborators. The codes `HIPR` and `PRF` [CG94] are provided for maximum flow, with the proviso that `HIPR` is recommended in most cases. For minimum-cost flow, the code of choice is `CS` [Gol97]. Both are written in C and available for noncommercial use from *http://www.avglab.com/andrew/soft.html*.

GOBLIN (*http://www.math.uni-augsburg.de/~fremuth/goblin.html*) is an extensive C++ library dealing with all of the standard graph optimization problems, including several different algorithms for both maximum flow and minimum-cost flow. The same holds true for LEDA, if a commercial-strength solution is needed. See Section 19.1.1 (page 658).

The First DIMACS Implementation Challenge on Network Flows and Matching [JM93] collected several implementations and generators for network flow, which can be obtained by anonymous FTP from *dimacs.rutgers.edu* in the directory *pub/netflow/maxflow*. These include: (1) a preflow-push network flow implementation in C by Edward Rothberg, and (2) an implementation of eleven network flow variants in C, including the older Dinic and Karzanov algorithms by Richard Anderson and Joao Setubal.

Notes: The primary book on network flows and its applications is [AMO93]. Good expositions on network flow algorithms old and new include [CCPS98, CLRS01, PS98]. Expositions on the hardness of multicommodity flow [Ita78] include [Eve79a].

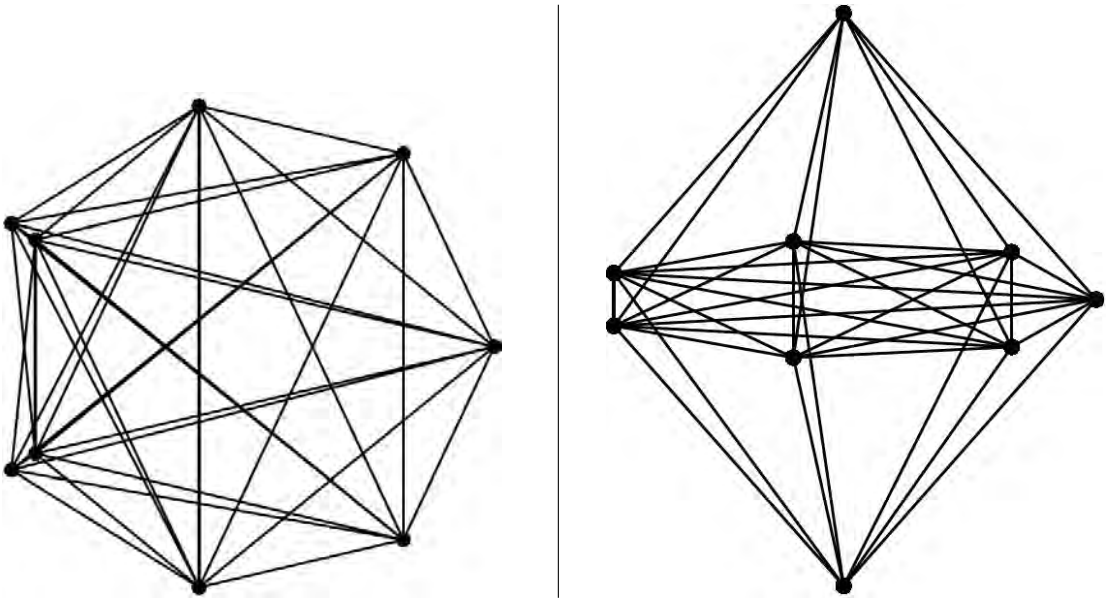
There is a very close connection to maximum flow and edge connectivity in graphs. The fundamental maximum-flow, minimum-cut theorem is due to Ford and Fulkerson

[FF62]. See Section 15.8 (page 505) for simpler and more efficient algorithms to compute the minimum cut in a graph.

Conventional wisdom holds that network flow should be computable in $O(nm)$ time, and there has been steady progress in lowering the time complexity. See [AMO93] for a history of algorithms for the problem. The fastest known general network flow algorithm runs in $O(nm \lg(n^2/m))$ time [GT88]. Empirical studies of minimum-cost flow algorithms include [GKK74, Gol97].

Information flows through a network can be modeled as multicommodity flows through a network, with the observation that replicating and manipulating information at internal nodes can eliminate the need for distinct sources to sink paths when multiple sinks are interested in the same information. The field of *network coding* [YLCZ05] uses such ideas to achieve information flows through networks at the theoretical limits of the max-flow, min-cut theorem.

Related Problems: Linear programming (see page 411), matching (see page 498), connectivity (see page 505).



INPUT OUTPUT

15.10 Drawing Graphs Nicely

Input description: A graph G.

Problem description: Draw a graph G so as to accurately reflect its structure.

Discussion: Graph drawing is a problem that constantly arises in applications, yet it is inherently ill-defined. What exactly does a nice drawing mean? We seek an algorithm that shows off the structure of the graph so the viewer can best understand it. Simultaneously, we seek a drawing that looks aesthetically pleasing.

Unfortunately, these are "soft" criteria for which it is impossible to design an optimization algorithm. Indeed, it is easy to come up with radically different drawings of a given graph, each of which is most appropriate in a certain context. Three different drawings of the Petersen graph are given on page 550. Which of these is the "right" one?

Several "hard" criteria can partially measure the quality of a drawing:

- *Crossings* – We seek a drawing with as few pairs of crossing edges as possible, since they are distracting.

- *Area* – We seek a drawing that uses as little paper as possible, while ensuring that no pair of vertices gets placed too close to each other.
- *Edge length* – We seek a drawing that avoids long edges, since they tend to obscure other features of the drawing.
- *Angular resolution* – We seek a drawing avoiding small angles between two edges incident on a given vertex, as the resulting lines tend to partially or fully overlap.
- *Aspect ratio* – We seek a drawing whose aspect ratio (width/height) reflects the desired output medium (typically a computer screen at 4/3) as closely as possible.

Unfortunately, these goals are mutually contradictory, and the problem of finding the best drawing under any nonempty subset of them is likely to be NP-complete.

Two final warnings before getting down to business. For graphs without inherent symmetries or structure, it is likely that no really nice drawing exists. This is especially for true for graphs with more than 10 to 15 vertices. The shear amount of ink needed to draw any large, dense graph will overwhelm any display. A drawing of the complete graph on 100 vertices (K_{100}) contains approximately 5,000 edges. On a 1000×1000 pixel display, this works out to 200 pixels per edge. What can you hope to see except a black blob in the center of the screen?

Once all this is understood, it must be admitted that graph-drawing algorithms can be quite effective and fun to play with. To help choose the right one, ask yourself the following questions:

- *Must the edges be straight, or can I have curves and/or bends?* – Straight-line drawing algorithms are relatively simple, but have their limitations. Orthogonal polyline drawings seem to work best to visualize complicated graphs such as circuit designs. *Orthogonal* means that all lines must be drawn either horizontal or vertical, with no intermediate slopes. *Polyline* means that each graph edge is represented by a chain of straight-line segments, connected by vertices or bends.
- *Is there a natural, application-specific drawing?* – If your graph represents a network of cities and roads, you are unlikely to find a better drawing than placing the vertices in the same position as the cities on a map. This same principle holds for many different applications.
- *Is your graph either planar or a tree?* – If so, use one of the special planar graph or tree drawing algorithms of Sections 15.11 and 15.12.
- *Is your graph directed?* – Edge direction has a significant impact on the nature of the desired drawing. When drawing directed acyclic graphs (DAGs), it is often important that all edges flow in a logical direction—perhaps left-right or top-down.

- *How fast must your algorithm be?* – Your graph drawing algorithm had better be very fast if it will be used for interactive update and display. You are presumably limited to using incremental algorithms, which change the vertex positions only in the immediate neighborhood of the edited vertex. You can afford more time for optimization if instead you are printing a pretty picture for extended study.

- *Does your graph contain symmetries?* – The output drawing above is attractive because the graph contains symmetries—namely two vertices identically connected to a core K_5. The inherent symmetries in a graph can be identified by computing its *automorphisms*, or self-isomorphisms. Graph isomorphism codes (see Section 16.9 (page 550)) can be readily used to find all automorphisms.

As a first quick and dirty drawing, I recommend simply spacing the vertices evenly on a circle, and then drawing the edges as straight lines between vertices. Such drawings are easy to program and fast to construct. They have the substantial advantage that no two edges will obscure each other, since no three vertices will be collinear. Such artifacts can be hard to avoid as soon as you allow internal vertices into your drawing. An unexpected pleasure with circular drawings is the symmetry sometimes revealed because vertices appear in the order they were inserted into the graph. Simulated annealing can be used to permute the circular vertex order to minimize crossings or edge length, and thus significantly improve the drawing.

A good, general purpose graph-drawing heuristic models the graph as a system of springs and then uses energy minimization to space the vertices. Let adjacent vertices attract each other with a force proportional to (say) the logarithm of their separation, while all nonadjacent vertices repel each other with a force proportional to their separation distance. These weights provide incentive for all edges to be as short as possible, while spreading the vertices apart. The behavior of such a system can be approximated by determining the force acting on each vertex at a particular time and then moving each vertex a small amount in the appropriate direction. After several such iterations, the system should stabilize on a reasonable drawing. The input and output figures above demonstrate the effectiveness of the spring embedding on a particular small graph.

If you need a polyline graph-drawing algorithm, my recommendation is that you study the systems presented next or described in [JM03] to decide whether one of them can do the job. You will have to do a significant amount of work before you can hope to develop a better algorithm.

Drawing your graph opens another can of worms, namely where to place the edge/vertex labels. We seek to position labels very close to the edges or vertices they identify, and yet to place them such that they do not overlap each other or other important graph features. Optimizing label placement can be shown to be an NP-complete problem, but heuristics related to bin packing (see Section 17.9 (page 595)) can be effectively used.

Implementations: GraphViz (*http://www.graphviz.org*) is a popular and well-supported graph-drawing program developed by Stephen North of Bell Laboratories. It represents edges as splines and can construct useful drawings of quite large and complicated graphs. It has sufficed for all of my professional graph-drawing needs over the years.

All of the graph data structure libraries of Section 12.4 (page 381) devote some effort to visualizing graphs. The Boost Graph Library provides an interface to GraphViz instead of reinventing the wheel. The Java graph libraries, most notably JGraphT (*http://jgrapht.sourceforge.net/*), are particularly suitable for interactive applications.

Graph drawing is a problem where very good commercial products exist, including those from Tom Sawyer Software (*www.tomsawyer.com*), yFiles (*www.yworks.com*), and iLOG's JViews (*www.ilog.com/products/jviews/*). Pajek [NMB05] is a package particularly designed for drawing social networks, and available at *http://vlado.fmf.uni-lj.si/pub/networks/pajek/*. All of these have free trial or noncommercial use downloads.

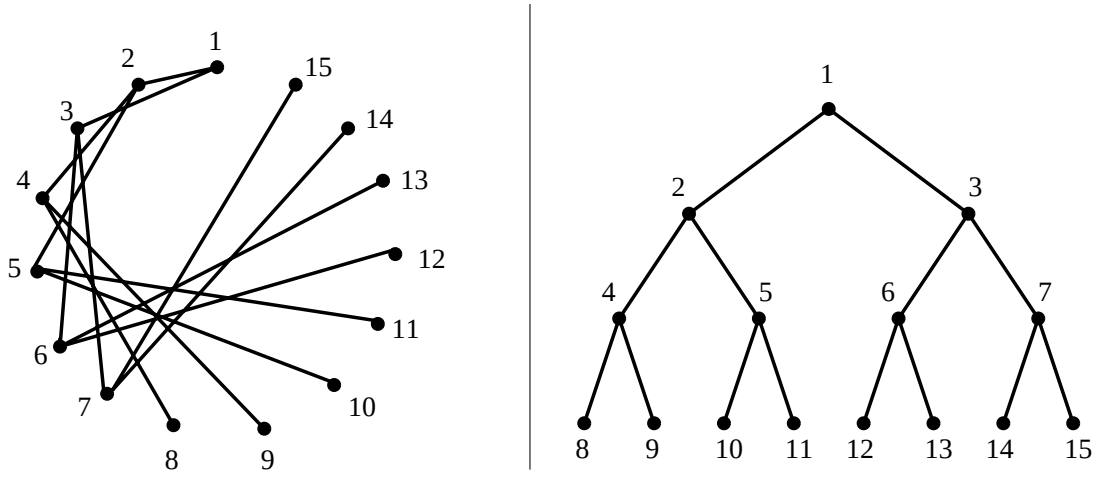
Combinatorica [PS03] provides Mathematica implementations of several graph-drawing algorithms, including circular, spring, and ranked embeddings. See Section 19.1.9 (page 661) for further information on Combinatorica.

Notes: A significant community of researchers in graph drawing exists, fueled by or fueling an annual conference on graph drawing. The proceedings of this conference are published by Springer-Verlag's Lecture Notes in Computer Science series. Perusing a volume of the proceedings will provide a good view of the state-of-the-art and of what kinds of ideas people are thinking about. The forthcoming *Handbook of Graph Drawing and Visualization* [Tam08] promises to be the most comprehensive review of the field.

Two excellent books on graph-drawing algorithms are Battista, et al. [BETT99] and Kaufmann and Wagner [KW01]. A third book by Jünger and Mutzel [JM03] is organized around systems instead of algorithms, but provides technical details about the drawing methods each system employs. Map-labeling heuristics are described in [BDY06, WW95].

It is trivial to space n points evenly along the boundary of a circle. However, the problem is considerably more difficult on the surface of a sphere. Extensive tables of such spherical codes for $n \leq 130$ have been constructed by Hardin, Sloane, and Smith [HSS07].

Related Problems: Drawing trees (see page 517), planarity testing (see page 520).



INPUT OUTPUT

15.11 Drawing Trees

Input description: A tree T, which is a graph without any cycles.

Problem description: Create a nice drawing of the tree T.

Discussion: Many applications require drawing pictures of trees. Tree diagrams are commonly used to display and traverse the hierarchical structure of file system directories. My attempts to Google "tree drawing software" revealed special-purpose applications for visualizing family trees, syntax trees (sentence diagrams), and evolutionary phylogenic trees all in the top twenty links.

Different aesthetics follow from each application. That said, the primary issue in tree drawing is establishing whether you are drawing free or rooted trees:

- *Rooted trees* define a hierarchical order, emanating from a single source node identified as the root. Any drawing should reflect this hierarchical structure, as well as any additional application-dependent constraints on the order in which children must appear. For example, family trees are rooted, with sibling nodes typically drawn from left to right in the order of birth.

- *Free trees* do not encode any structure beyond their connection topology. There is no root associated with the minimum spanning tree (MST) of a graph, so a hierarchical drawing will be misleading. Such free trees might well inherit their drawing from that of the full underlying graph, such as the map of the cities whose distances define the MST.

Trees are always planar graphs, and hence can and should be drawn so no two edges cross. Any of the planar drawing algorithms of Section 15.12 (page 520) could be used to do so. However, such algorithms are overkill, because much simpler algorithms can be used to construct planar drawings of trees. The spring-embedding heuristics of Section 15.10 (page 513) work well on free trees, although they may be too slow for certain applications.

The most natural tree-drawing algorithms assume rooted trees. However, they can be used equally well with free trees, after selecting one vertex to serve as the root of the drawing. This faux-root can be selected arbitrarily, or, even better, by using a *center* vertex of the tree. A center vertex minimizes the maximum distance to other vertices. For trees, the center always consists of either one vertex or two adjacent vertices. This tree center can be identified in linear time by repeatedly trimming all the leaves until only the center remains.

Your two primary options for drawing rooted trees are *ranked* and *radial* embeddings:

- *Ranked embeddings* – Place the root in the top center of your page, and then partition the page into the root-degree number of top-down strips. Deleting the root creates the root-degree number of subtrees, each of which is assigned to its own strip. Draw each subtree recursively, by placing its new root (the vertex adjacent to the old root) in the center of its strip a fixed distance down from the top, with a line from old root to new root. The output figure above is a nicely ranked embedding of a balanced binary tree.

  Such ranked embeddings are particularly effective for rooted trees used to represent a hierarchy—be it a family tree, data structure, or corporate ladder. The top-down distance illustrates how far each node is from the root. Unfortunately, such repeated subdivision eventually produces very narrow strips, until most of the vertices are crammed into a small region of the page. Try to adjust the width of each strip to reflect the total number of nodes it will contain, and don't be afraid of expanding into neighboring region's turf once their shorter subtrees have been completed.

- *Radial embeddings* – Free trees are better drawn using a radial embedding, where the root/center of the tree is placed in the center of the drawing. The space around this center vertex is divided into angular sectors for each subtree. Although the same problem of cramping will eventually occur, radial embeddings make better use of space than ranked embeddings and appear considerably more natural for free trees. The rankings of vertices in terms of distance from the center is illustrated by the concentric circles of vertices.

Implementations: GraphViz (*http://www.graphviz.org*) is a popular and well-supported graph-drawing program developed by Stephen North of Bell Laboratories. It represents edges as splines and can construct useful drawings of quite large

and complicated graphs. It has sufficed for all of my professional graph drawing needs over the years.

Graph/tree drawing is a problem where very good commercial products exist, including those from Tom Sawyer Software (*www.tomsawyer.com*), yFiles (*www.yworks.com*), and iLOG's JViews (*www.ilog.com/products/jviews/*). All of these have free trial or noncommercial use downloads.

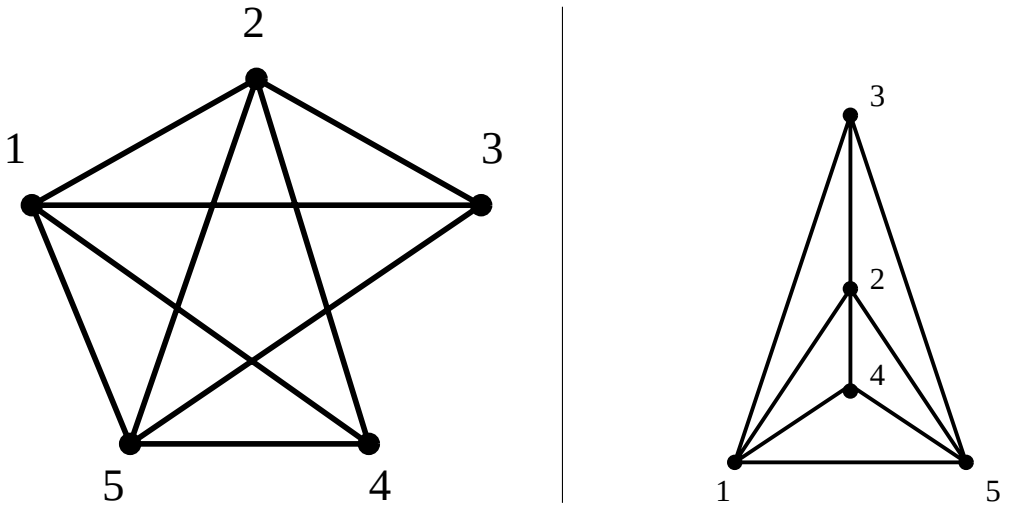
Combinatorica [PS03] provides Mathematica implementations of several tree drawing algorithms, including radial and rooted embeddings. See Section 19.1.9 (page 661) for further information on Combinatorica.

Notes: All books and surveys on graph drawing include discussions of specific tree-drawing algorithms. The forthcoming *Handbook of Graph Drawing and Visualization* [Tam08] promises to be the most comprehensive review of the field. Two excellent books on graph drawing algorithms are Battista, et al. [BETT99] and Kaufmann and Wagner [KW01]. A third book by Jünger and Mutzel [JM03] is organized around systems instead of algorithms, but provides technical details about the drawing methods each system employs.

Heuristics for tree layout have been studied by several researchers [RT81, Moe90], with Buchheim, et al. [BJL06] reflective of the state-of-the-art. Under certain aesthetic criteria, the problem is NP-complete [SR83].

Certain tree layout algorithms arise from non-drawing applications. The Van Emde Boas layout of a binary tree offers better external memory performance than conventional binary search, at a cost of greater complexity. See the survey of Arge, et al. [ABF05] for more on this and other cache-oblivious data structures.

Related Problems: Drawing graphs (see page 513), planar drawings (see page 520).



INPUT OUTPUT

15.12 Planarity Detection and Embedding

Input description: A graph G.

Problem description: Can G be drawn in the plane such that no two edges cross? If so, produce such a drawing.

Discussion: Planar drawings (or *embeddings*) make clear the structure of a given graph by eliminating crossing edges, which can be confused as additional vertices. Graphs defined by road networks, printed circuit board layouts, and the like are inherently planar because they are completely defined by surface structures.

Planar graphs have a variety of nice properties that can be exploited to yield faster algorithms for many problems. The most important fact to know is that every planar graph is *sparse*. Euler's formula shows that $|E| \leq 3|V| - 6$ for every nontrivial planar graph $G = (V, E)$. This means that every planar graph contains a linear number of edges, and further that every planar graph contains a vertex of degree ≤ 5. Every subgraph of a planar graph is planar, so there must always a sequence of low-degree vertices to delete from G, reducing it to the empty graph.

To gain a better appreciation of the subtleties of planar drawings, I encourage the reader to construct a planar (noncrossing) embedding for the graph $K_5 - e$, shown on the input figure above. Then try to construct such an embedding where all the edges are straight. Finally, add the missing edge to the graph and try to do the same for K_5 itself.

The study of planarity has motivated much of the development of graph theory. It must be confessed, however, that the need for planarity testing arises relatively infrequently in applications. Most graph-drawing systems do not explicitly seek planar embeddings. *"Planarity Detection"* proved to be among the least frequently hit pages of the Algorithm Repository (*http://www.cs.sunysb.edu/∼algorith*) [Ski99]. That said, it is still very useful to know how to deal with planar graphs when you encounter them.

Thus, it pays to distinguish the problem of planarity testing (does a graph have a planar drawing?) from constructing planar embeddings (actually finding the drawing), although both can be done in linear time. Many efficient planar graph algorithms do not make any use of the drawing, but instead exploit the low-degree deletion sequence described above.

Algorithms for planarity testing begin by embedding an arbitrary cycle from the graph in the plane and then considering additional paths in G, connecting vertices on this cycle. Whenever two such paths cross, one must be drawn outside the cycle and one inside. When three such paths mutually cross, there is no way to resolve the problem, so the graph cannot be planar. Linear-time algorithms for planarity detection are based on depth-first search, but they are subtle and complicated enough that you are wise to seek an existing implementation.

Such path-crossing algorithms can be used to construct a planar embedding by inserting the paths into the drawing one by one. Unfortunately, because they work in an incremental manner, nothing prevents them from inserting many vertices and edges into a relatively small area of the drawing. Such cramping is a major problem, for it leads to ugly drawings that are hard to understand. Better algorithms have been devised that construct *planar-grid embeddings*, where each vertex lies on a $(2n - 4) \times (n - 2)$ grid. Thus, no region can get too cramped and no edge can get too long. Still, the resulting drawings tend not to look as natural as one might hope.

For nonplanar graphs, what is often sought is a drawing that minimizes the number of crossings. Unfortunately, computing the crossing number of a graph is NP-complete. A useful heuristic extracts a large planar subgraph of G, embeds this subgraph, and then inserts the remaining edges one by one to minimize the number of crossings. This won't do much for dense graphs, which are doomed to have a large number of crossings, but it will work well for graphs that are almost planar, such as road networks with overpasses or printed circuit boards with multiple layers. Large planar subgraphs can be found by modifying planarity-testing algorithms to delete troublemaking edges when encountered.

Implementations: LEDA (see Section 19.1.1 (page 658)) includes linear-time algorithms for both planarity testing and constructing straight-line planar-grid embeddings. Their planarity tester returns an obstructing Kuratowski subgraph (see notes) for any graph deemed nonplanar, yielding concrete proof of its nonplanarity.

JGraphEd (*http://www.jharris.ca/JGraphEd/*) is a Java graph-drawing framework that includes several planarity testing/embedding algorithms, including both the Booth-Lueker PQ-tree algorithm and the modern straight-line grid embedding.

PIGALE (*http://pigale.sourceforge.net/*) is a C++ graph editor/algorithm library focusing on planar graphs. It contains a variety of algorithms for constructing planar drawings as well as efficient algorithms to test planarity and identify an obstructing subgraph ($K_{3,3}$ or K_5), if one exists.

Greedy randomized adaptive search (GRASP) heuristics for finding the largest planar subgraph have been implemented by Ribeiro and Resende [RR99] as Algorithm 797 of the *Collected Algorithms of the ACM* (see Section 19.1.6 (page 659)). These Fortran codes are also available from *http://www.research.att.com/∼mgcr/src/*.

Notes: Kuratowski [Kur30] gave the first characterization of planar graphs, namely that they do not contain a subgraph homeomorphic to $K_{3,3}$ or K_5. Thus, if you are still working on the exercise to embed K_5, now is an appropriate time to give it up. Fary's theorem [FÁ48] states that every planar graph can be drawn in such a way that each edge is straight.

Hopcroft and Tarjan [HT74] gave the first linear-time algorithm for drawing graphs. Booth and Lueker [BL76] developed an alternate planarity-testing algorithm based on PQ-trees. Simplified planarity-testing algorithms include [BCPB04, MM96, SH99]. Efficient $2n \times n$ planar grid embeddings were first developed by [dFPP90]. The book by Nishizeki and Rahman [NR04] provide a good overview of the spectrum of planar drawing algorithms.

Outerplanar graphs are those that can be drawn so all vertices lie on the outer face of the drawing. Such graphs can be characterized as having no subgraph homeomorphic to $K_{2,3}$ and can be recognized and embedded in linear time.

Related Problems: Graph partition (see page 541), drawing trees (see page 517).

16

Graph Problems: Hard Problems

A cynical view of graph algorithms is that "everything we want to do is hard." Indeed, no polynomial-time algorithms are known for any of the problems in this section. All of them are provably NP-complete with the exception of graph isomorphism—whose complexity status remains an open question.

The theory of NP-completeness demonstrates that *all* NP-complete problems must have polynomial-time algorithms if *any* one of them does. This prospect is sufficiently preposterous that an NP-completeness reduction suffices as de facto proof that no efficient algorithm exists to solve the given problem.

Still, do not abandon hope if your problem resides in this chapter. We provide a recommended line of attack for each problem, be it combinatorial search, heuristics, approximation algorithms, or algorithms for restricted instances. Hard problems require a different methodology to work with than polynomial-time problems, but with care they can usually be dealt with successfully.

The following books will help you deal with NP-complete problems:

- *Garey and Johnson* [GJ79] – This is the classic reference on the theory of NP-completeness. Most notably, it contains a concise catalog of over 400 NP-complete problems, with associated references and comments. Browse through the catalog as soon as you question the existence of an efficient algorithm for your problem. Indeed, this is the single book in my library that I reach for most often.

- *Crescenzi and Kann* [ACG+03] – This book serves as the "Garey and Johnson" for the world of approximation algorithms. Its reference section, *The Compendium of NP Optimization Problems*, is maintained online at *www.nada.kth.se/∼viggo/problemlist/* and should be the first place to look for a provably good heuristic for any given problem.

S.S. Skiena, *The Algorithm Design Manual*, 2nd ed., DOI: 10.1007/978-1-84800-070-4_16,
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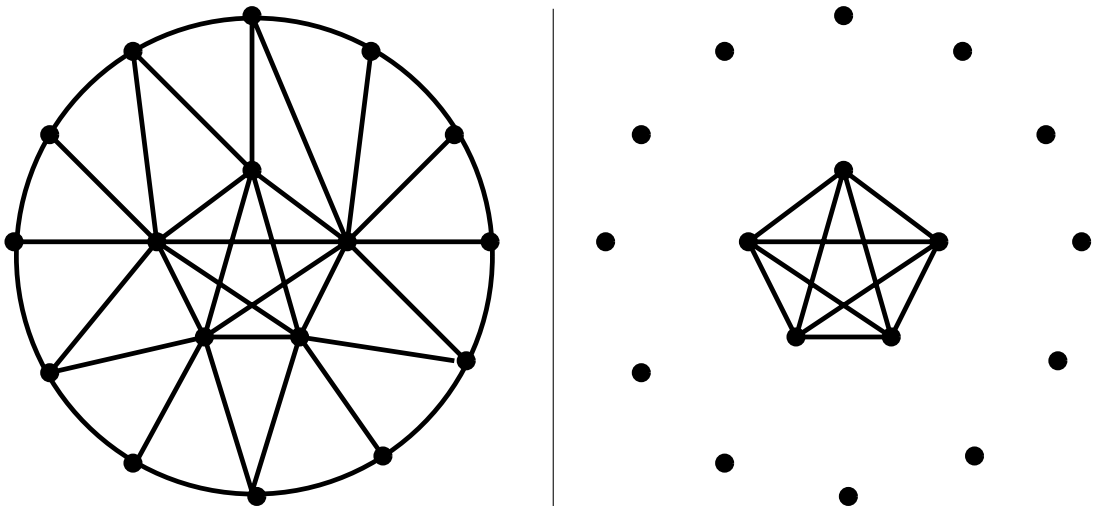
- *Vazirani* [Vaz04] – A complete treatment of the theory of approximation algorithms by a highly regarded researcher in the field.
- *Hochbaum* [Hoc96] – This nice book was the first survey of approximation algorithms for NP-complete problems, but rapid developments have left it somewhat dated.
- *Gonzalez* [Gon07] – This *Handbook of Approximation Algorithms and Metaheuristics* contains current surveys on a variety of techniques for dealing with hard problems, both applied and theoretical.



INPUT OUTPUT

16.1 Clique

Input description: A graph $G = (V, E)$.

Problem description: What is the largest $S \subset V$ such that for all $x, y \in S$, $(x, y) \in E$?

Discussion: In high school, everybody complained about the "clique,"—a group of friends who all hung around together and seemed to dominate everything social. Consider a graph representing the school's social network. Vertices correspond to people, with edges between any pair of people who are friends. Thus, the high school clique defines a (complete subgraph) clique in this friendship graph.

Identifying "clusters" of related objects often reduces to finding large cliques in graphs. An interesting example arose in a program the Internal Revenue Service (IRS) developed to detect organized tax fraud. In this scam, large groups of phony tax returns are submitted in the hopes of getting undeserved refunds. But generating large numbers of *different* phony tax returns is hard work. The IRS constructs graphs with vertices corresponding to submitted tax forms and edges between any two forms that appear suspiciously similar. Any large clique in this graph points to fraud.

Since any edge in a graph represents a clique of two vertices, the challenge lies not in finding a clique, but in finding a large clique. And it is indeed a challenge, for finding a maximum clique is NP-complete. To make matters worse, it is provably

hard to approximate even to within a factor of $n^{1/2-\epsilon}$. Theoretically, clique is about as hard as a problem in this book can get. So what can we hope to do about it?

- *Will a maximal clique suffice?* – A *maximal* clique is a clique that cannot be enlarged by adding any additional vertex. This doesn't mean that it has to be large relative to the largest possible clique, but it might be. To find a nice maximal (and hopefully large) clique, sort the vertices from highest degree to lowest degree, put the first vertex in the clique, and then test each of the other vertices to see whether it is adjacent to all the clique vertices added thus far. If so, add it; if not, continue down the list. By using a bit vector to mark which vertices are currently in the clique, this can be made to run in $O(n+m)$ time. An alternative approach might incorporate some randomness into the vertex ordering, and accept the largest maximal clique you find after a certain number of trials.

- *What if I will settle for a large, dense subgraph?* – Insisting on cliques to define clusters in a graph can be risky, since a single missing edge will eliminate a vertex from consideration. Instead, we should seek large *dense* subgraphs—i.e. , subsets of vertices that contain a large number of edges between them. Cliques are, by definition, the densest subgraphs possible.

  The largest set of vertices whose induced (defined) subgraph has minimum vertex degree $\geq k$ can be found with a simple linear-time algorithm. Begin by deleting all the vertices whose degree is less than k. This may reduce the degree of other vertices below k, if they were adjacent to sufficiently deleted low-degree vertices. Repeating this process until all remaining vertices have degree $\geq k$ constructs the largest high-degree subgraph. This algorithm can be implemented in $O(n+m)$ time by using adjacency lists and the constant-width priority queue of Section 12.2 (page 373). If we continue to delete the lowest-degree vertices, we eventually end up with a clique or set of cliques, – but they may be as small as two vertices.

- *What if the graph is planar?* – Planar graphs cannot have cliques of a size larger than four, or else they cease to be planar. Since each edge defines a clique of size 2, the only interesting cases are cliques of three and four vertices. Efficient algorithms to find such small cliques consider the vertices from lowest to highest degree. Any planar graph must contain a vertex of at most 5 degrees (see Section 15.12 (page 520)), so there is only a constant-sized neighborhood to check exhaustively for a clique containing it. We then delete this vertex to leave a smaller planar graph, containing another low-degree vertex. Repeat this check and delete processes until the graph is empty.

If you *really* need to find the largest clique in a graph, an exhaustive search via backtracking provides the only real solution. We search through all k-subsets of the vertices, pruning a subset as soon as it contains a vertex that is not adjacent to all the rest. A simple upper bound on the maximum clique in G is the highest vertex

degree plus 1. A better upper bound comes from sorting the vertices in order of decreasing degree. Let j be the largest index such that degree of the jth vertex is at least $j-1$. The largest clique in the graph contains no more than j vertices, since no vertex of degree $< (j-1)$ can appear in a clique of size j. To speed our search, we should delete all such useless vertices from G.

Heuristics for finding large cliques based on randomized techniques such as simulated annealing are likely to work reasonably well.

Implementations: `Cliquer` is a set of C routines for finding cliques in arbitrary weighted graphs by Patric Östergard. It uses an exact branch-and-bound algorithm, and is available at *http://users.tkk.fi/~pat/cliquer.html*.

Programs for finding cliques and independent sets were sought for the Second DIMACS Implementation Challenge [JT96]. Programs and data from the challenge are available by anonymous FTP from *dimacs.rutgers.edu*. Source codes are available under *pub/challenge/graph* and test data under *pub/djs*. `dfmax.c` implements a simple-minded branch-and-bound algorithm similar to [CP90]. `dmclique.c` uses a "semi-exhaustive greedy" scheme for finding large independent sets from [JAMS91].

Kreher and Stinson [KS99] provide branch-and-bound programs in C for finding the maximum clique using a variety of lower-bounds, available at *http://www.math.mtu.edu/~kreher/cages/Src.html*.

GOBLIN (*http://www.math.uni-augsburg.de/~fremuth/goblin.html*) implements branch-and-bound algorithms for finding large cliques. They claim to be able to work with graphs as large as 150 to 200 vertices.

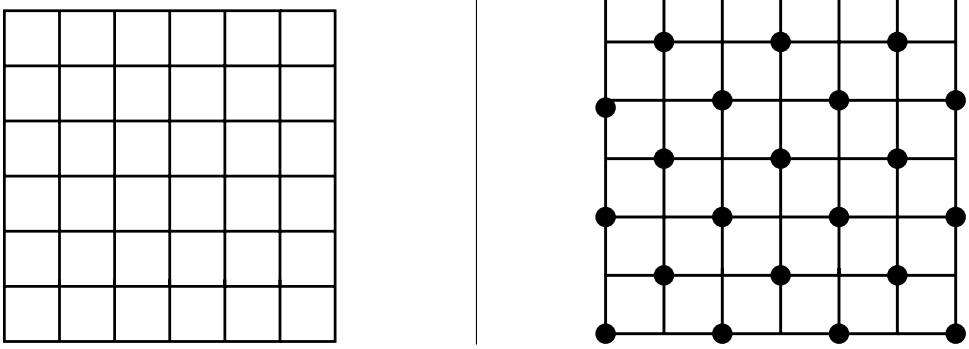
Notes: Bomze, et al. [BBPP99] give the most comprehensive survey on the problem of finding maximum cliques. Particularly interesting is the work from the operations research community on branch-and-bound algorithms for finding cliques effectively. More recent experimental results are reported in [JS01].

The proof that clique is NP-complete is due to Karp [Kar72]. His reduction (given in Section 9.3.3 (page 327)) established that clique, vertex cover, and independent set are very closely related problems, so heuristics and programs that solve one of them should also produce reasonable solutions for the other two.

The *densest subgraph problem* seeks the subset of vertices whose induced subgraph has the highest average vertex degree. A clique of k vertices is clearly the densest subgraph of its size, but larger, noncomplete subgraphs may achieve higher average degree. The problem is NP-complete, but simple heuristics based on repeatedly deleting the lowest-degree vertex achieve reasonable approximation ratios [AITT00]. See [GKT05] for an interesting application of densest subgraph, namely detecting link spam on the Web.

That clique cannot be approximated to within a factor of $n^{1/2-\epsilon}$ unless $P = NP$ (and $n^{1-\epsilon}$ under weaker assumptions) is shown in [Has82].

Related Problems: Independent set (see page 528), vertex cover (see page 530).



INPUT OUTPUT

16.2 Independent Set

Input description: A graph $G = (V, E)$.

Problem description: What is the largest subset S of vertices of V such that for each edge $(x, y) \in E$, either $x \notin E$ or $y \notin E$?

Discussion: The need to find large independent sets arises in facility dispersion problems, where we seek a set of mutually separated locations. It is important that no two locations of our new "McAlgorithm" franchise service be placed close enough to compete with each other. We can construct a graph where the vertices are the set of possible locations, and then add edges between any two locations deemed close enough to interfere. The maximum independent set gives the largest number of franchises we can sell without cannibalizing sales.

Independent sets (also known as *stable sets*) avoid conflicts between elements, and hence arise often in coding theory and scheduling problems. Define a graph whose vertices represent the set of possible code words, and add edges between any two code words sufficiently similar to be confused due to noise. The maximum independent set of this graph defines the highest capacity code for the given communication channel.

Independent set is closely related to two other NP-complete problems:

- *Clique* – Watch what you say, for a clique is what you get if you give an independent set a complement. The *complement* of $G = (V, E)$ is a graph $G' = (V, E')$ where $(i, j) \in E'$ iff (i, j) is not in E. In other words, we replace each edge by a non-edge and vice versa. The maximum independent set in G is exactly the maximum clique in G', so the two problems are algorithmically

identical. Thus, the algorithms and implementations in Section 16.1 (page 525) can easily be used for independent set.

- *Vertex coloring* – The vertex coloring of a graph $G = (V, E)$ is a partition of V into a small number of sets (colors), where no two vertices of the same color can have an edge between them. Each color class defines an independent set. Many scheduling applications of independent set are really coloring problems, since all tasks eventually must be completed.

  Indeed, one heuristic to find a large independent set is to use any vertex coloring algorithm/heuristic, and take the largest color class. One consequence of this observation is that all graphs with small chromatic numbers (such as planar and bipartite graphs) have large independent sets.

The simplest reasonable heuristic is to find the lowest-degree vertex, add it to the independent set, and then delete it and all vertices adjacent to it. Repeating this process until the graph is empty gives a *maximal* independent set, in that it can't be made larger by just adding vertices. Using randomization or perhaps some degree of exhaustive search might result in somewhat larger independent sets.

The independent set problem is in some sense dual to the graph-matching problem. The former asks for a large set of vertices with no edge in common, while the latter asks for a large set of edges with no vertex in common. This suggests trying to rephrase your problem as an efficiently-computable matching problem instead of maximum independent set problem, which is NP-complete.

The maximum independent set of a tree can be found in linear time by (1) stripping off the leaf nodes, (2) adding them to the independent set, (3) deleting all adjacent nodes, and then (4) repeating from the first step on the resulting trees until it is empty.

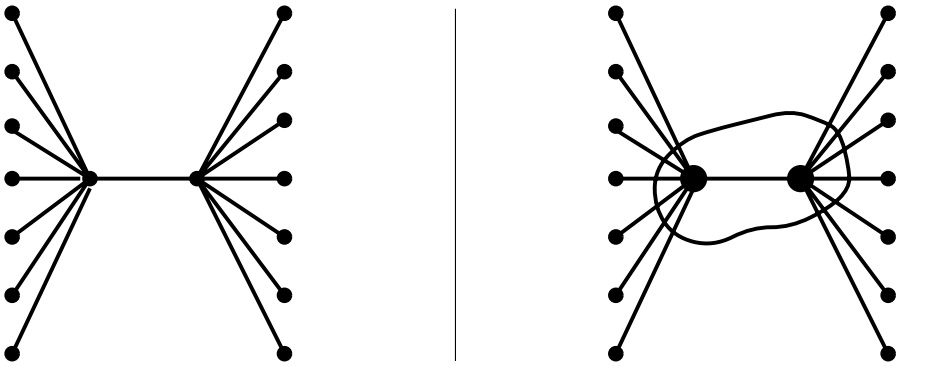
Implementations: Any program for computing the maximum clique in a graph can find maximum independent sets by just complementing the input graph. Therefore, we refer the reader to the clique-finding programs of Section 16.1 (page 525).

GOBLIN (*http://www.math.uni-augsburg.de/~fremuth/goblin.html*) implements a branch-and-bound algorithm for finding independent sets (called stable sets in the manual).

Greedy randomized adaptive search (GRASP) heuristics for independent set set have been implemented by Resende, et al. [RFS98] as Algorithm 787 of the *Collected Algorithms of the ACM* (see Section 19.1.6 (page 659)). These Fortran codes are also available from *http://www.research.att.com/~mgcr/src/*.

Notes: The proof that independent set is NP-complete is due to Karp [Kar72]. It remains NP-complete for planar cubic graphs [GJ79]. Independent set can be solved efficiently for bipartite graphs [Law76]. This is not trivial—indeed the larger of the "part" of a bipartite graph is not necessarily its maximum independent set.

Related Problems: Clique (see page 525), vertex coloring (see page 544), vertex cover (see page 530).



INPUT OUTPUT

16.3 Vertex Cover

Input description: A graph $G = (V, E)$.

Problem description: What is the smallest subset of $S \subset V$ such that each edge $(x, y) \in E$ contains at least one vertex of S?

Discussion: Vertex cover is a special case of the more general *set cover* problem, which takes as input an arbitrary collection of subsets $S = (S_1, \ldots, S_n)$ of the universal set $U = \{1, \ldots, m\}$. We seek the smallest subset of subsets from S whose union is U. Set cover arises in many applications associated with buying things sold in fixed lots or assortments. See Section 18.1 (page 621) for a discussion of set cover.

To turn vertex cover into a set cover problem, let universal set U represent the set E of edges from G, and define S_i to be the set of edges incident on vertex i. A set of vertices defines a vertex cover in graph G iff the corresponding subsets define a set cover in this particular instance. However, since each edge can be in only two different subsets, vertex cover instances are simpler than general set cover. Vertex cover is a relative lightweight among NP-complete problems, and can be more effectively solved than general set cover.

Vertex cover and independent set are very closely related graph problems. Since every edge in E is (by definition) incident on a vertex in any cover S, there can be no edge both endpoints are in $V - S$. Thus, $V - S$ must be an independent set. Since minimizing S is the same as maximizing $V - S$, the problems are equivalent. This means that any independent set solver can be applied to vertex cover as well. Having two ways of looking at your problem is helpful, since one may appear easier in a given context.

The simplest heuristic for vertex cover selects the vertex with highest degree, adds it to the cover, deletes all adjacent edges, and then repeats until the graph is empty. With the right data structures, this can be done in linear time, and should "usually" produce a "pretty good" cover. However, this cover might be $\lg n$ times worse than the optimal cover for certain input graphs.

Fortunately, we can always find a vertex cover whose size is at most twice as large as optimal. Find a *maximal* matching M in the graph—i.e. , a set of edges no two of which share a vertex in common and which cannot be enlarged by adding additional edges. Such a maximal matching can be constructed incrementally, by picking an arbitrary edge e in the graph, deleting any edge sharing a vertex with e, and repeating until the graph is out of edges. Taking *both* of the vertices for each edge in a maximal matching gives us a vertex cover. Why? Because *any* vertex cover must contain *at least* one of the two vertices in each matching edge just to cover the edges of M, this cover is at most twice as large as the minimum cover.

This heuristic can be tweaked to perform somewhat better in practice, if not in theory. We can select the matching edges to "kill off" as many other edges as possible, which should reduce the size of the maximal matching and hence the number of pairs of vertices in the vertex cover. Also, some of the vertices from M may in fact not be necessary, since all of their incident edges might also have been covered using other selected vertices. We can identify and delete these losers by making a second pass through our cover.

The vertex cover problem seeks to cover all edges using few vertices. Two other important problems have similar sounding objectives:

- *Cover all vertices using few vertices* – The *dominating set* problem seeks the smallest set of vertices D such that every vertex in $V - D$ is adjacent to at least one vertex in the dominating set D. Every vertex cover of a nontrivial connected graph is also a dominating set, but dominating sets can be much smaller. Any single vertex represents the minimum dominating set of complete graph K_n, while $n-1$ vertices are needed for a vertex cover. Dominating sets tend to arise in communications problems, since they represent the hubs or broadcast centers sufficient to communicate with all sites/users.

  Dominating set problems can be easily expressed as instances of set cover (see Section 18.1 (page 621)). Each vertex v_i defines a subset of vertices consisting of itself plus all the vertices it is adjacent to. The greedy set cover heuristic running on this instance yields a $\Theta(\lg n)$ approximation to the optimal dominating set.

- *Cover all vertices using few edges* – The *edge cover* problem seeks the smallest set of edges such that each vertex is included in one of the edges. In fact, edge cover can be solved efficiently by finding a maximum cardinality matching (see Section 15.6 (page 498)) and then selecting arbitrary edges to account for the unmatched vertices.

Implementations: Any program for computing the maximum clique in a graph can be applied to vertex cover by complementing the input graph and selecting the vertices which do not appear in the clique. Therefore, we refer the reader to check out the clique-finding programs of Section 16.1 (page 525).

`COVER` [RHG07] is a very effective vertex cover solver based on a stochastic local search algorithm. It is available at *http://www.nicta.com.au/people/richters/*.

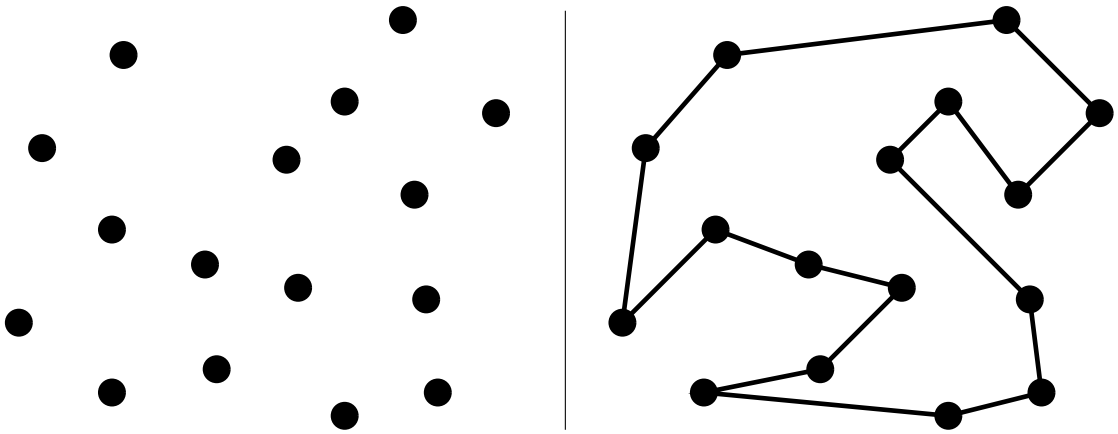
JGraphT (*http://jgrapht.sourceforge.net/*) is a Java graph library that contains greedy and 2-approximate heuristics for vertex cover.

Notes: Karp [Kar72] first proved that vertex-cover is NP-complete. Several different heuristics yield 2-approximation algorithms for vertex cover, including randomized rounding. Good expositions on these 2-approximation algorithms include [CLRS01, Hoc96, Pas97, Vaz04]. The example that the greedy algorithm can be as bad as $\lg n$ times optimal is due to [Joh74] and presented in [PS98]. Experimental studies of vertex cover heuristics include [GMPV06, GW97, RHG07].

Whether there exists a better than 2-factor approximation for vertex cover is one of the major open problems in approximation algorithms. Hastad [Has97] proved there does not exist a better than 1.1666-factor approximation algorithm for vertex cover.

The primary reference on dominating sets is the monograph of Haynes et al. [HHS98]. Heuristics for the connected dominating set problem are presented in [GK98]. Dominating set cannot be approximated to better than the $\Omega(\lg n)$ factor [ACG+03] of set cover.

Related Problems: Independent set (see page 528), set cover (see page 621).



INPUT OUTPUT

16.4 Traveling Salesman Problem

Input description: A weighted graph G.

Problem description: Find the cycle of minimum cost, visiting each vertex of G exactly once.

Discussion: The traveling salesman problem is the most notorious NP-complete problem. This is a function both of its general usefulness and the ease with which it can be explained to the public at large. Imagine a traveling salesman planning a car trip to visit a set of cities. What is the shortest route that will enable him to do so and return home, thus minimizing his total driving?

The traveling salesman problem arises in many transportation and routing problems. Other important applications involve optimizing tool paths for manufacturing equipment. For example, consider a robot arm assigned to solder all the connections on a printed circuit board. The shortest tour that visits each solder point exactly once defines the most efficient route for the robot.

Several issues arise in solving TSPs:

- *Is the graph unweighted?* – If the graph is unweighted, or all the edges have one of two possible cost values, the problem reduces to finding a *Hamiltonian cycle*. See Section 16.5 (page 538) for a discussion of this problem.

- *Does your input satisfy the triangle inequality?* – Our sense of how proper distance measures behave is captured by the *triangle inequality*. This property states that $d(i, j) \leq d(i, k) + d(k, j)$ for all vertices $i, j, k \in V$. Geometric

distances all satisfy the triangle inequality because the shortest distance between two points is as the crow flies. Commercial air fares do *not* satisfy the triangle inequality, which is why it is so hard to find the cheapest airfare between two points. TSP heuristics work much better on sensible graphs that do obey the triangle inequality.

- *Are you given n points as input or a weighted graph?* – Geometric instances are often easier to work with than a graph representation. Since pair of points define a complete graph, there is never an issue of finding a feasible tour. We can save space by computing these distances on demand, thus eliminating the need to store an $n \times n$ distance matrix. Geometric instances inherently satisfy the triangle inequality, so they can exploit performance guarantees from certain heuristics. Finally, one can take advantage of geometric data structures like kd-trees to quickly identify close unvisited sites.

- *Can you visit a vertex more than once?* – The restriction that the tour not revisit any vertex is irrelevant in many applications. In air travel, the cheapest way to visit all vertices might involve repeatedly visiting an airport hub. Note that this issue does not arise when the input observes the triangle inequality.

  TSP with repeated vertices is easily solved by using any conventional TSP code on a new cost matrix D, where $D(i, j)$ is the shortest path distance from i to j. This matrix can be constructed by solving an all-pairs shortest path (see Section 15.4 (page 489)) and satisfies the triangle inequality.

- *Is your distance function symmetric?* – A distance function is *asymmetric* when there exists x, y such that $d(x, y) \neq d(y, x)$. The asymmetric traveling salesman problem (ATSP) is much harder to solve in practice than symmetric (STSP) instances. Try to avoid such pathological distance functions. Be aware that there is a reduction converting ATSP instances to symmetric instances containing twice as many vertices [GP07], that may be useful because symmetric solvers are so much better.

- *How important is it to find the optimal tour?* – Usually heuristic solutions will suffice for applications. There are two different approaches if you insist on solving your TSP to optimality, however. *Cutting plane methods* model the problem as an integer program, then solve the linear programming relaxation of it. Additional constraints designed to force integrality are added if the optimal solution is not at an integer point. *Branch-and-bound algorithms* perform a combinatorial search while maintaining careful upper and lower bounds on the cost of a tour. In the hands of professionals, problems with thousands of vertices can be solved. Maybe you can too, if you use the best solver available.

Almost any flavor of TSP is going to be NP-complete, so the right way to proceed is with heuristics. These typically come within a few percent of the optimal

solution, which is close enough for engineering work. Unfortunately, literally dozens of heuristics have been proposed for TSP, so the situation can be confusing. Empirical results in the literature are sometime contradictory. However, we recommend choosing from among the following heuristics:

- *Minimum spanning trees* – This heuristic starts by finding the minimum spanning tree (MST) of the sites, and then does a depth-first search of the resulting tree. In the course of DFS, we walk over each of the $n-1$ edges exactly twice: once going down to discover a new vertex, and once going up when we backtrack. Now define a tour by ordering the vertices by when they were discovered. If the graph obeys the triangle inequality, the resulting tour is at most twice the length of the optimal TSP tour. In practice, it is usually better, typically 15% to 20% over optimal. Furthermore, the running time is bounded by that of computing the MST, which is only $O(n \lg n)$ in the case of points in the plane (see Section 15.3 (page 484)).

- *Incremental insertion methods* – A different class of heuristics starts from a single vertex, and then inserts new points into this partial tour one at a time until the tour is complete. The version of this heuristic that seems to work best is *furthest point* insertion: of all remaining points, insert the point v into a partial tour T such that

  $$\max_{v \in V} \min_{i=1}^{|T|} (d(v, v_i) + d(v, v_{i+1}))$$

  The "min" ensures that we insert the vertex in the position that adds the smallest amount of distance to the tour, while the "max" ensures that we pick the worst such vertex first. This seems to work well because it "roughs out" a partial tour first before filling in details. Such tours are typically only 5% to 10% longer than optimal.

- *K-optimal tours* – Substantially more powerful are the Kernighan-Lin, or *k-opt*, class of heuristics. The method applies local refinements to an initially arbitrary tour in the hopes of improving it. In particular, subsets of k edges are deleted from the tour and the k remaining subchains rewired to form a different tour with hopefully a better cost. A tour is k-optimal when no subset of k edges can be deleted and rewired to reduce the cost of the tour. Two-opting a tour is a fast and effective way to improve any other heuristic. Extensive experiments suggest that 3-optimal tours are usually within a few percent of the cost of optimal tours. For $k > 3$, the computation time increases considerably faster than the solution quality. Simulated annealing provides an alternate mechanism to employ edge flips to improve heuristic tours.

Implementations: Concorde is a program for the symmetric traveling salesman problem and related network optimization problems, written in ANSI C. This

world record-setting program by Applegate, Bixby, Chvatal, and Cook [ABCC07] has obtained the optimal solutions to 106 of TSPLIB's 110 instances; the largest of which has 15,112 cities. Concorde is available for academic research use from *http://www.tsp.gatech.edu/concorde*. It is the clear choice among available TSP codes. Their *http://www.tsp.gatech.edu/* website features very interesting material on the history and applications of TSP.

Lodi and Punnen [LP07] put together an excellent survey of available software for solving TSP. Current links to all programs mentioned are maintained at *http://www.or.deis.unibo.it/research_pages/tspsoft.html*.

TSPLIB [Rei91] provides the standard collection of hard instances of TSPs that arise in practice. The best-supported version of TSPLIB is available from *http://www.iwr.uni-heidelberg.de/groups/comopt/software/TSPLIB95/*, although the instances are also available from Netlib (see Section 19.1.5 (page 659)).

Tsp_solve is a C++ code by Chad Hurwitz and Robert Craig that provides both heuristic and optimal solutions. Geometric problems of size up to 100 points are manageable. It is available from *http://www.cs.sunysb.edu/∼algorith* or by e-mailing Chad Hurrwitz at churritz@cts.com. GOBLIN (*http://www.math.uni-augsburg.de/∼fremuth/goblin.html*) implements branch-and-bound algorithms for both symmetric and asymmetric TSP, as well as a variety of heuristics.

Algorithm 608 [Wes83] of the *Collected Algorithms of the ACM* is a Fortran implementation of a heuristic for the quadratic assignment problem—a more general problem that includes the traveling salesman as a special case. Algorithm 750 [CDT95] is a Fortran code for the exact solution of asymmetric TSP instances. See Section 19.1.5 (page 659) for details.

Notes: The book by Applegate, Bixby, Chvatal, and Cook [ABCC07] documents the techniques they used in their record-setting TSP solvers, as well as the theory and history behind the problem. Gutin and Punnen [GP07] now offer the best reference on all aspects and variations of the traveling salesman problem, displacing an older but much beloved book by Lawler et al. [LLKS85].

Experimental results on heuristic methods for solving large TSPs include [Ben92a, GBDS80, Rei94]. Typically, it is possible to get within a few percent of optimal with such methods.

The Christofides heuristic [Chr76] is an improvement over the minimum-spanning tree heuristic and guarantees a tour whose cost is at most 3/2 times optimal on Euclidean graphs. It runs in $O(n^3)$, where the bottleneck is the time it takes to find a minimum-weight perfect matching (see Section 15.6 (page 498)). The minimum spanning tree heuristic is due to [RSL77].

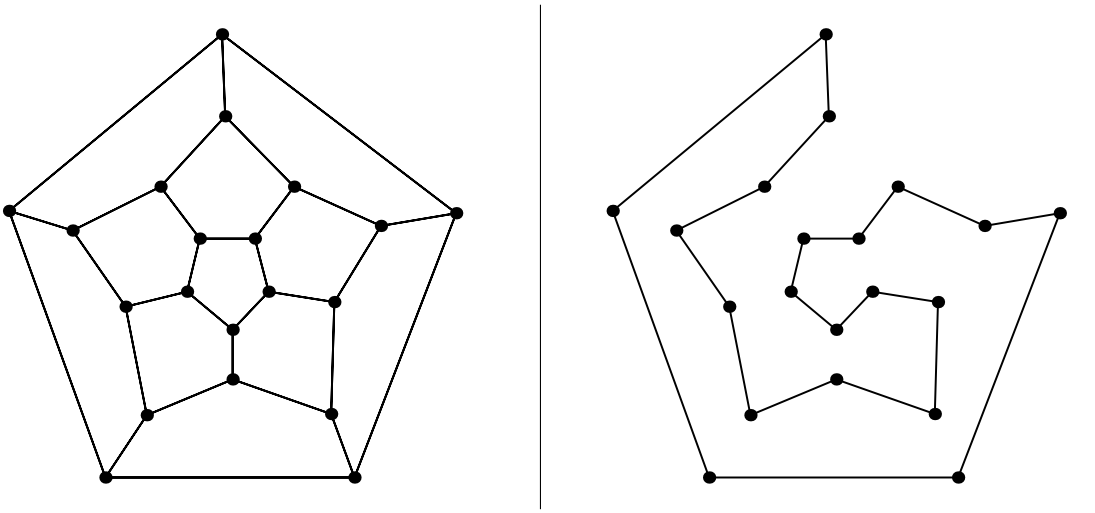
Polynomial-time approximation schemes for Euclidean TSP have been developed by Arora [Aro98] and Mitchell [Mit99], which offer $1 + \epsilon$ factor approximations in polynomial time for any $\epsilon > 0$. They are of great theoretical interest, although any practical consequences remain to be determined.

The history of progress on optimal TSP solutions is inspiring. In 1954, Dantzig, Fulkerson, and Johnson solved a symmetric TSP instance of 42 United States cities [DFJ54]. In 1980, Padberg and Hong solved an instance on 318 vertices [PH80]. Applegate et al. [ABCC07] have recently solved problems that are twenty times larger than this. Some of

this increase is due to improved hardware, but most is due to better algorithms. The rate of growth demonstrates that exact solutions to NP-complete problems can be obtained for large instances if the stakes are high enough. Fortunately or unfortunately, they seldom are.

Size is not the only criterion for hard instances. One can easily construct an enormous graph consisting of one cheap cycle, for which it would be easy to find the optimal solution. For sets of points in convex position in the plane, the minimum TSP tour is described by its convex hull (see Section 17.2 (page 568)), which can be computed in $O(n \lg n)$ time. Other easy special cases are known.

Related Problems: Hamiltonian cycle (see page 538), minimum spanning tree (see page 484), convex hull (see page 568).



INPUT OUTPUT

16.5 Hamiltonian Cycle

Input description: A graph $G = (V, E)$.

Problem description: Find a tour of the vertices using only edges from G, such that each vertex is visited exactly once.

Discussion: Finding a Hamiltonian cycle or path in a graph G is a special case of the traveling salesman problem G'—one where each edge in G has distance 1 in $'G$. Non-edge vertex pairs are separated by a greater distance, say 2. Such a weighted graph has TSP tour of cost n in G' iff G is Hamiltonian.

Closely related is the problem of finding the longest path or cycle in a graph. This arises often in pattern recognition problems. Let the vertices in the graph correspond to possible symbols, with edges linking pairs of symbols that might occur next to each other. The longest path through this graph is a good candidate for the proper interpretation.

The problems of finding longest cycles and paths are both NP-complete, even on very restrictive classes of unweighted graphs. There are several possible lines of attack, however:

- *Is there a serious penalty for visiting vertices more than once?* – Reformulating the Hamiltonian cycle problem instead of minimizing the total number of vertices visited on a complete tour turns it into an optimization problem.

This allows possibilities for heuristics and approximation algorithms. Finding a spanning tree of the graph and doing a depth-first search, as discussed in Section 16.4 (page 533), yields a tour with at most $2n$ vertices. Using randomization or simulated annealing might bring the size of this down considerably.

- *Am I seeking the longest path in a directed acyclic graph (DAG)?* – The problem of finding the longest path in a DAG can be solved in linear time using dynamic programming. Conveniently, the algorithm for finding the *shortest* path in a DAG (presented in Section 15.4 (page 489)) does the job if we replace min with max. DAGs are the most interesting case of longest path for which efficient algorithms exist.

- *Is my graph dense?* – Sufficiently dense graphs always contain Hamiltonian cycles. Further, the cycles implied by such sufficiency conditions can be efficiently constructed. In particular, any graph where all vertices have degree $\geq n/2$ must be Hamiltonian. Stronger sufficient conditions also hold; see the Notes section.

- *Are you visiting all the vertices or all the edges?* – Verify that you really have a vertex-tour problem and not an edge-tour problem. With a little cleverness it is sometimes possible to reformulate a Hamiltonian cycle problem in terms of Eulerian cycles, which instead visit every edge of a graph. Perhaps the most famous such instance is the problem of constructing de Bruijn sequences, discussed in Section 15.7 (page 502). The benefit is that fast algorithms exist for Eulerian cycles and many related variants, while Hamiltonian cycle is NP-complete.

If you *really* must know whether your graph is Hamiltonian, backtracking with pruning is your only possible solution. Certainly check whether your graph is biconnected (see Section 15.8 (page 505)). If not, this means that the graph has an articulation vertex whose deletion will disconnect the graph and so cannot be Hamiltonian.

Implementations: The construction described above (weight 1 for an edge and 2 for a non-edge) reduces Hamiltonian cycles to a symmetric TSP problem that obeys the triangle inequality. Thus we refer the reader to the TSP solvers discussed in Section 16.4 (page 533). Foremost among them is `Concorde`, a program for the symmetric traveling salesman problem and related network optimization problems, written in ANSI C. `Concorde` is available for academic research use from *http://www.tsp.gatech.edu/concorde*. It is the clear choice among available TSP codes.

An effective program for solving Hamiltonian cycle problems resulted from the masters thesis of Vandegriend [Van98]. Both the code and the thesis are available from *http://web.cs.ualberta.ca/∼joe/Theses/vandegriend.html*.

Lodi and Punnen [LP07] put together an excellent survey of available TSP software, including the special case of Hamiltonian cycle. Current links to all programs are maintained at *http://www.or.deis.unibo.it/research_pages/tspsoft.html*.

The football program of the Stanford GraphBase (see Section 19.1.8 (page 660)) uses a stratified greedy algorithm to solve the asymmetric longest-path problem. The goal is to derive a chain of football scores to establish the superiority of one football team over another. After all, if Virginia beat Illinois by 30 points, and Illinois beat Stony Brook by 14 points, then by transitivity Virginia would beat Stony Brook by 44 points if they played, right? We seek the longest simple path in a graph where the weight of edge (x, y) denotes the number of points by which x beat y.

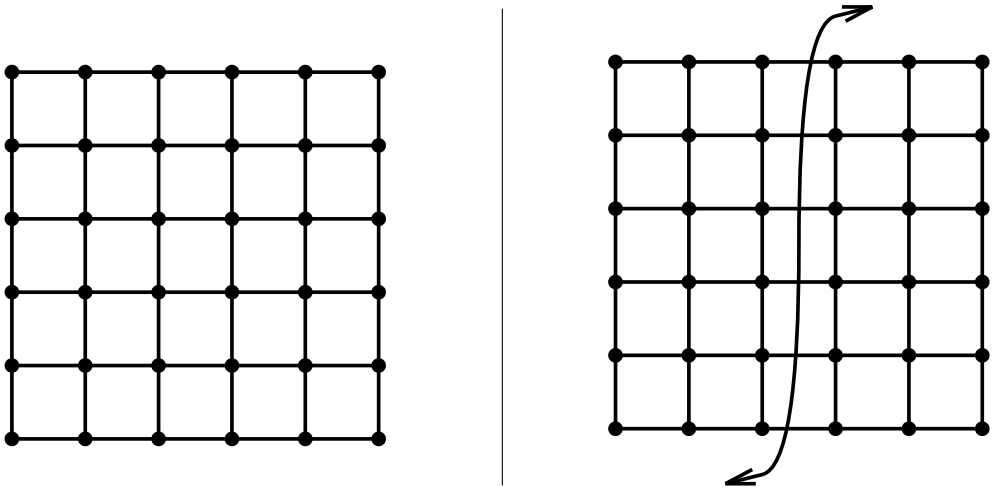
Nijenhuis and Wilf [NW78] provide an efficient routine to enumerate all Hamiltonian cycles of a graph by backtracking. See Section 19.1.10 (page 661). Algorithm 595 [Mar83] of the *Collected Algorithms of the ACM* is a similar Fortran code that can be used as either an exact procedure or a heuristic by controlling the amount of backtracking. See Section 19.1.5 (page 659).

Notes: Hamiltonian cycles apparently first arose in Euler's study of the knight's tour problem, although they were popularized by Hamilton's "Around the World" game in 1839. See [ABCC07, GP07, LLKS85] for comprehensive references on the traveling salesman problem, including discussions on Hamiltonian cycle.

Most good texts in graph theory review sufficiency conditions for graphs to be Hamiltonian. My favorite is West [Wes00].

Techniques for solving optimization problems in the laboratory using biological processes have attracted considerable attention. In the original application of these "biocomputing" techniques, Adleman [Adl94] solved a seven-vertex instance of the directed Hamiltonian path problem. Unfortunately, this approach requires an exponential number of molecules, and Avogadro's number implies that such experiments are inconceivable for graphs beyond $n \approx 70$.

Related Problems: Eulerian cycle (see page 502), traveling salesman (see page 533).



INPUT OUTPUT

16.6 Graph Partition

Input description: A (weighted) graph $G = (V, E)$ and integers k and m.

Problem description: Partition the vertices into m roughly equal-sized subsets such that the total edge cost spanning the subsets is at most k.

Discussion: Graph partitioning arises in many divide-and-conquer algorithms, which gain their efficiency by breaking problems into equal-sized pieces such that the respective solutions can easily be reassembled. Minimizing the number of edges cut in the partition usually simplifies the task of merging.

Graph partition also arises when we need to cluster the vertices into logical components. If edges link "similar" pairs of objects, the clusters remaining after partition should reflect coherent groupings. Large graphs are often partitioned into reasonable-sized pieces to improve data locality or make less cluttered drawings.

Finally, graph partition is a critical step in many parallel algorithms. Consider the finite element method, which is used to compute the physical properties (such as stress and heat transfer) of geometric models. Parallelizing such calculations requires partitioning the models into equal-sized pieces whose interface is small. This is a graph-partitioning problem, since the topology of a geometric model is usually represented using a graph.

Several different flavors of graph partitioning arise depending on the desired objective function:

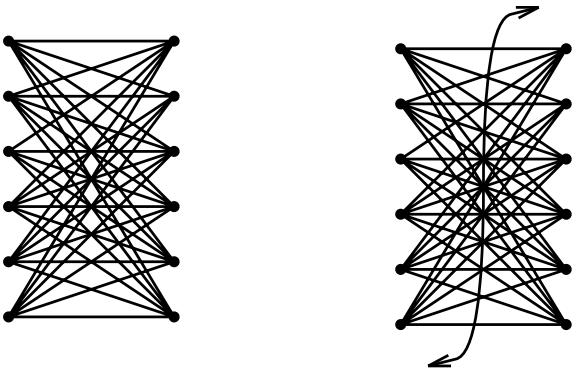


Figure 16.1: The maximum cut of a graph

- *Minimum cut set* – The *smallest* set of edges to cut that will disconnect a graph can be efficiently found using network flow or randomized algorithms. See Section 15.8 (page 505) for more on connectivity algorithms. The smallest cutset might split off only a single vertex, so the resulting partition could be very unbalanced.

- *Graph partition* – A better partition criterion seeks a small cut that partitions the vertices into roughly equal-sized pieces. Unfortunately, this problem is NP-complete. Fortunately, the heuristics discussed below work well in practice.

  Certain special graphs always have small *separators*, that partition the vertices into balanced pieces. For any tree, there always exists a single vertex whose deletion partitions the tree so that no component contains more than $n/2$ of the original n vertices. These components need not always be connected; consider the separating vertex of a star-shaped tree. This separating vertex can be found in linear time using depth first-search. Every planar graph has a set of $O(\sqrt{n})$ vertices whose deletion leaves no component with more than $2n/3$ vertices. These separators provide a useful way to decompose geometric models, which are often defined by planar graphs.

- *Maximum cut* – Given an electronic circuit specified by a graph, the *maximum cut* defines the largest amount of data communication that can simultaneously occur in the circuit. The highest-speed communications channel should thus span the vertex partition defined by the maximum edge cut. Finding the maximum cut in a graph is NP-complete [Kar72], however heuristics similar to those of graph partitioning work well.

The basic approach for dealing with graph partitioning or max-cut problems is to construct an initial partition of the vertices (either randomly or according

to some problem-specific strategy) and then sweep through the vertices, deciding whether the size of the cut would improve if we moved this vertex over to the other side. The decision to move vertex v can be made in time proportional to its degree, by identifying which side of the partition contains more of v's neighbors. Of course, the desirable side for v may change after its neighbors jump, so several iterations are likely to be needed before the process converges on a local optimum. Even so, such a local optimum can be arbitrarily far away from the global max-cut.

There are many variations of this basic procedure, by changing the order we test the vertices in or moving clusters of vertices simultaneously. Using some form of randomization, particularly simulated annealing, is almost certain to be a good idea. When more than two components are desired, the partitioning heuristic should be applied recursively.

Spectral partitioning methods use sophisticated linear algebra techniques to obtain a good partitioning. The spectral bisection method uses the second-lowest eigenvector of the *Laplacian matrix* of the graph to partition it into two pieces. Spectral methods tend to do a good job of identifying the general area to partition, but the results can be improved by cleaning up with a local optimization method.

Implementations: Chaco is a widely-used graph partitioning code designed to partition graphs for parallel computing applications. It employs several different partitioning algorithms, including both Kernighan-Lin and spectral methods. Chaco is available at *http://www.cs.sandia.gov/~bahendr/chaco.html*.

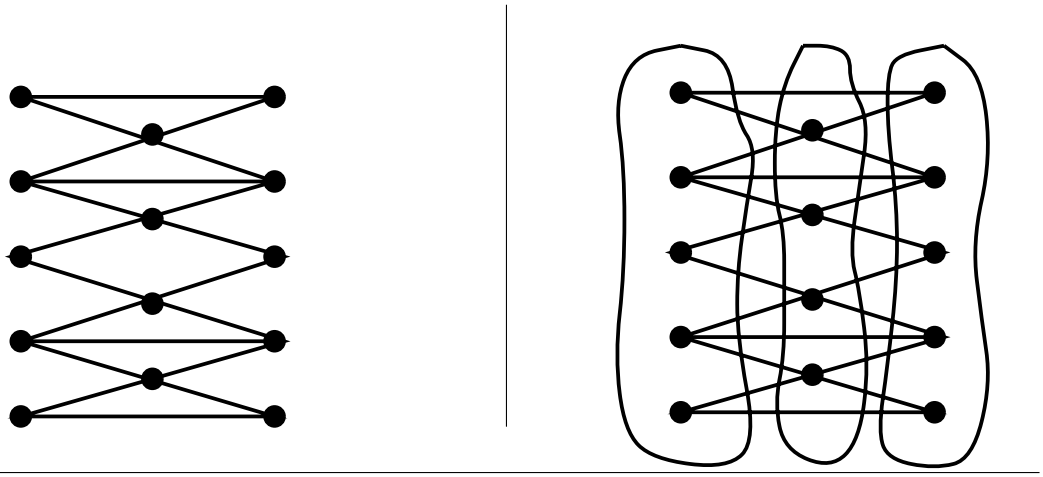
METIS (*http://glaros.dtc.umn.edu/gkhome/views/metis*) is another well-regarded code for graph partitioning. It has successfully partitioned graphs with over 1,000,000 vertices. Available versions include one variant designed to run on parallel machines and another suitable for partitioning hypergraphs. Other respected codes include Scotch (*http://www.labri.fr/perso/pelegrin/scotch/*) and JOSTLE (*http://staffweb.cms.gre.ac.uk/~wc06/jostle/*).

Notes: The fundamental local improvement heuristics for graph partitioning are due to Kernighan-Lin [KL70] and Fiduccia-Mattheyses [FM82]. Spectral methods for graph partition are discussed in [Chu97, PSL90]. Empirical results on graph partitioning heuristics include [BG95, LR93].

The planar separator theorem and an efficient algorithm for finding such a separator are due to Lipton and Tarjan [LT79, LT80]. For experiences in implementing planar separator algorithms, see [ADGM04, HPS+05].

Any random vertex partition will expect to cut half of the edges in the graph, since the probability that the two vertices defining an edge end up on different sides of the partition is 1/2. Goemans and Williamson [GW95] gave an 0.878-factor approximation algorithm for maximum-cut, based on semi-definite programming techniques. Tighter analysis of this algorithm was followed by Karloff [Kar96].

Related Problems: Edge/vertex connectivity (see page 505), network flow (see page 509).



INPUT OUTPUT

16.7 Vertex Coloring

Input description: A graph $G = (V, E)$.

Problem description: Color the vertices of V using the minimum number of colors such that i and j have different colors for all $(i, j) \in E$.

Discussion: Vertex coloring arises in many scheduling and clustering applications. Register allocation in compiler optimization is a canonical application of coloring. Each variable in a given program fragment has a range of times during which its value must be kept intact, in particular after it is initialized and before its final use. Any two variables whose life spans intersect cannot be placed in the same register. Construct a graph where each vertex corresponds to a variable, with an edge between any two vertices whose variable life spans intersect. Since none of the variables assigned the same color clash, they all can be assigned to the same register.

No conflicts will occur if each vertex is colored using a distinct color. But computers have a limited number of registers, so we seek a coloring using the fewest colors. The smallest number of colors sufficient to vertex-color a graph is its *chromatic number*.

Several special cases of interest arise in practice:

- *Can I color the graph using only two colors?* – An important special case is testing whether a graph is *bipartite*, meaning it can be colored using only two different colors. Bipartite graphs arise naturally in such applications as mapping workers to possible jobs. Fast, simple algorithms exist for problems

such as matching (see Section 15.6 (page 498)) when restricted to bipartite graphs.

Testing whether a graph is bipartite is easy. Color the first vertex blue, and then do a depth-first search of the graph. Whenever we discover a new, uncolored vertex, color it opposite of its parent, since the same color would cause a clash. The graph cannot be bipartite if we ever find an edge (x, y) where both x and y have been colored identically. Otherwise, the final coloring will be a 2-coloring, constructed in $O(n + m)$ time. An implementation of this algorithm is given in Section 5.7.2 (page 167).

- *Is the graph planar, or are all vertices of low degree?* – The famous four-color theorem states that every planar graph can be vertex colored using at most four distinct colors. Efficient algorithms for finding a four-coloring on planar graphs are known, although it is NP-complete to decide whether a given planar graph is three-colorable.

  There is a very simple algorithm to find a vertex coloring of a planar graph using at most six colors. In any planar graph, there exists a vertex of at most five degree. Delete this vertex and recursively color the graph. This vertex has at most five neighbors, which means that it can always be colored using one of the six colors that does not appear as a neighbor. This works because deleting a vertex from a planar graph leaves a planar graph, meaning that it must also have a low-degree vertex to delete. The same idea can be used to color any graph of maximum degree Δ using $\leq \Delta + 1$ colors in $O(n\Delta)$ time.

- *Is this an edge-coloring problem?* – Certain vertex coloring problems can be modeled as *edge coloring*, where we seek to color the edges of a graph G such that no two edges are colored the same if they have a vertex in common. The payoff is that there is an efficient algorithm that always returns a near-optimal edge coloring. Algorithms for edge coloring are the focus of Section 16.8 (page 548).

Computing the chromatic number of a graph is NP-complete, so if you need an exact solution you must resort to backtracking, which can be surprisingly effective in coloring certain random graphs. It remains hard to compute a good approximation to the optimal coloring, so expect no guarantees.

Incremental methods are the heuristic of choice for vertex coloring. As in the previously-mentioned algorithm for planar graphs, vertices are colored sequentially, with the colors chosen in response to colors already assigned in the vertex's neighborhood. These methods vary in how the next vertex is selected and how it is assigned a color. Experience suggests inserting the vertices in nonincreasing order of degree, since high-degree vertices have more color constraints and so are most likely to require an additional color if inserted late. Brèlaz's heuristic [Brè79] dynamically selected the uncolored vertex of highest *color degree* (i.e. , adjacent to the most different colors), and colors it with the lowest-numbered unused color.

Incremental methods can be further improved by using *color interchange*. Taking a properly colored graph and exchanging two of the colors (painting the red vertices blue and the blue vertices red) leaves a proper vertex coloring. Now suppose we take a properly colored graph and delete all but the red and blue vertices. We can repaint one or more of the resulting connected components, again leaving a proper coloring. After such a recoloring, some vertex v previously adjacent to both red and blue vertices might now be only adjacent to blue vertices, thus freeing v to be colored red.

Color interchange is a win in terms of producing better colorings, at a cost of increased time and implementation complexity. Implementations are described next. Simulated annealing algorithms that incorporate color interchange to move from state to state are likely to be even more effective.

Implementations: Graph coloring has been blessed with two useful Web resources. Culberson's graph coloring page, *http://web.cs.ualberta.ca/∼joe/Coloring/*, provides an extensive bibliography and programs to generate and solve hard graph coloring instances. Trick's page, *http://mat.gsia.cmu.edu/COLOR/color.html*, provides a nice overview of graph coloring applications, an annotated bibliography, and a collection of over 70 graph-coloring instances arising in applications such as register allocation and printed circuit board testing. Both contain a C language implementation of the DSATUR coloring algorithm.

Programs for the closely related problems of finding cliques and vertex coloring graphs were sought for at the Second DIMACS Implementation Challenge [JT96], held in October 1993. Programs and data from the challenge are available by anonymous FTP from *dimacs.rutgers.edu*. Source codes are available under *pub/challenge/graph* and test data under *pub/djs*, including a simple "semi-exhaustive greedy" scheme used in the graph-coloring algorithm XRLF [JAMS91].

GraphCol (*http://code.google.com/p/graphcol/*) contains tabu search and simulated annealing heuristics for constructing colorings in C.

The C++ Boost Graph Library [SLL02] (*http://www.boost.org/libs/graph/doc*) contains an implementation of greedy incremental vertex coloring heuristics. GOBLIN (*http://www.math.uni-augsburg.de/∼fremuth/goblin.html*) implements a branch-and-bound algorithm for vertex coloring.

Pascal implementations of backtracking algorithms for vertex coloring and several heuristics, including largest-first and smallest-last incremental orderings and color interchange, appear in [SDK83]. See Section 19.1.10 (page 662).

Nijenhuis and Wilf [NW78] provide an efficient Fortran implementation of chromatic polynomials and vertex coloring by backtracking. See Section 19.1.10 (page 661).

Combinatorica [PS03] provides Mathematica implementations of bipartite graph testing, heuristic colorings, chromatic polynomials, and vertex coloring by backtracking. See Section 19.1.9 (page 661).

Notes: An old but excellent source on vertex coloring heuristics is Syslo, Deo, and Kowalik [SDK83], which includes experimental results. Classical heuristics for vertex coloring include [Brè79, MMI72, Tur88]; see [GH06, HDD03] for more recent results.

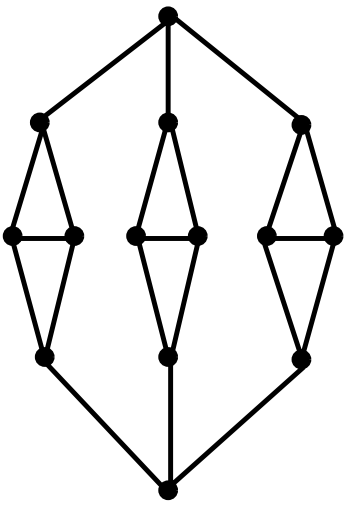
Wilf [Wil84] proved that backtracking to test whether a random graph has chromatic number k runs in *constant time*, dependent on k but independent of n. This is not as interesting as it sounds, because only a vanishingly small fraction of such graphs are indeed k-colorable. A number of provably efficient (but still exponential) algorithms for vertex coloring are known. See [Woe03] for a survey.

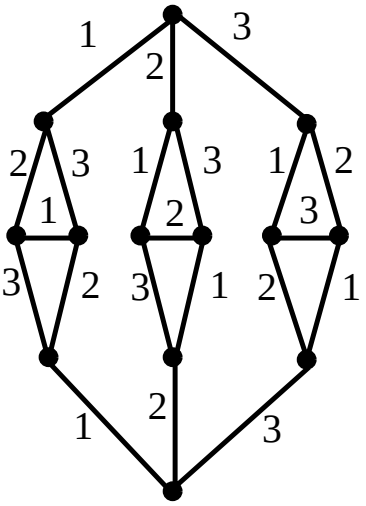
Paschos [Pas03] reviews what is known about provably good approximation algorithms for vertex coloring. On one hand, it is provably hard to approximate within a polynomial factor [BGS95]. On the other hand, there are heuristics that offer some nontrivial guarantees in terms of various parameters, such as Wigderson's [Wig83] factor of $n^{1-1/(\chi(G)-1)}$ approximation algorithm, where $\chi(G)$ is the chromatic number of G.

Brook's theorem states that the chromatic number $\chi(G) \leq \Delta(G) + 1$, where $\Delta(G)$ is the maximum degree of a vertex of G. Equality holds only for odd-length cycles (which have chromatic number 3) and complete graphs.

The most famous problem in the history of graph theory is the four-color problem, first posed in 1852 and finally settled in 1976 by Appel and Haken using a proof involving extensive computation. Any planar graph can be five-colored using a variation of the color interchange heuristic. Despite the four-color theorem, it is NP-complete to test whether a particular planar graph requires four colors or if three suffice. See [SK86] for an exposition on the history of the four-color problem and the proof. An efficient algorithm to four-color a graph is presented in [RSST96].

Related Problems: Independent set (see page 528), edge coloring (see page 548).





INPUT OUTPUT

16.8 Edge Coloring

Input description: A graph $G = (V, E)$.

Problem description: What is the smallest set of colors needed to color the edges of G such that no two same-color edges share a common vertex?

Discussion: The edge coloring of graphs arises in scheduling applications, typically associated with minimizing the number of noninterfering rounds needed to complete a given set of tasks. For example, consider a situation where we must schedule a given set of two-person interviews, where each interview takes one hour. All meetings could be scheduled to occur at distinct times to avoid conflicts, but it is less wasteful to schedule nonconflicting events simultaneously. We construct a graph whose vertices are people and whose edges represent the pairs of people who need to meet. An edge coloring of this graph defines the schedule. The color classes represent the different time periods in the schedule, with all meetings of the same color happening simultaneously.

The National Football League solves such an edge-coloring problem each season to make up its schedule. Each team's opponents are determined by the records of the previous season. Assigning the opponents to weeks of the season is an edge-coloring problem, complicated by extra constraints of spacing out rematches and making sure that there is a good game every Monday night.

The minimum number of colors needed to edge color a graph is called its *edge-chromatic number* by some and its *chromatic index* by others. Note that an even-length cycle can be edge-colored with 2 colors, while odd-length cycles have an edge-chromatic number of 3.

Edge coloring has a better (if less famous) theorem associated with it than vertex coloring. Vizing's theorem states that any graph with a maximum vertex degree of Δ can be edge colored using at most $\Delta + 1$ colors. To put this in perspective, note that *any* edge coloring must have at least Δ colors, since all the edges incident on any vertex must be distinct colors.

The proof of Vizing's theorem is constructive, meaning it can be turned into an $O(nm\Delta)$ algorithm to find an edge-coloring with $\Delta + 1$ colors. Since deciding whether we can get away using one less color than this is NP-complete, it hardly seems worth the effort to worry about it. An implementation of Vizing's theorem is described below.

Any edge-coloring problem on G can be converted to the problem of finding a vertex coloring on the *line graph* $L(G)$, which has a vertex of $L(G)$ for each edge of G and an edge of $L(G)$ if and only if the two edges of G share a common vertex. Line graphs can be constructed in time linear to their size, and any vertex-coloring code can be employed to color them. That said, it is disappointing to go the vertex coloring route. Vizing's theorem is our reward for the extra thought needed to see that we have an edge-coloring problem.

Implementations: Yan Dong produced an implementation of Vizing's theorem in C++ as a course project for my algorithms course while a student at Stony Brook. It can be found on the algorithm repository site at *http://www.cs.sunysb.edu/∼algorith*.

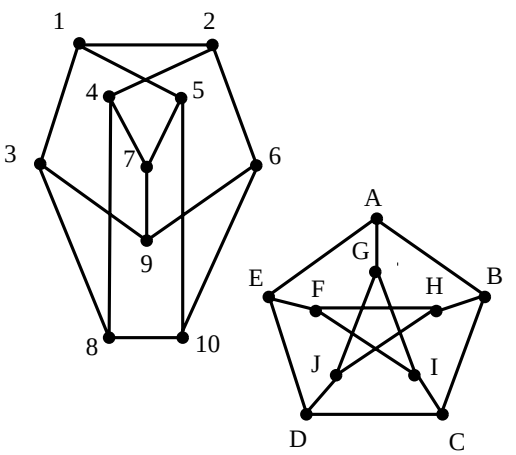
GOBLIN (*http://www.math.uni-augsburg.de/∼fremuth/goblin.html*) implements a branch-and-bound algorithm for edge coloring.

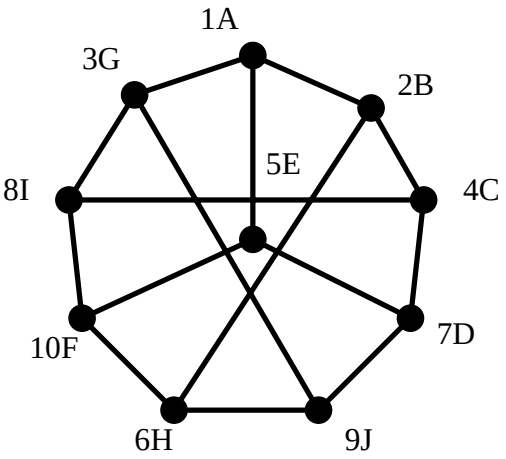
See Section 16.7 (page 544) for a larger collection of vertex-coloring codes and heuristics, which can be applied to the line graph of your target graph. Combinatorica [PS03] provides Mathematica implementations of edge coloring in this fashion, via the line graph transformation and vertex coloring routines. See Section 19.1.9 (page 661) for more information on Combinatorica.

Notes: Graph-theoretic results on edge coloring are surveyed in [FW77, GT94]. Vizing [Viz64] and Gupta [Gup66] independently proved that any graph can be edge colored using at most $\Delta + 1$ colors. Misra and Gries give a simple constructive proof of this result [MG92]. Despite these tight bounds, it is NP-complete to compute the edge-chromatic number [Hol81]. Bipartite graphs can be edge-colored in polynomial time [Sch98].

Whitney, in introducing line graphs [Whi32], showed that with the exception of K_3 and $K_{1,3}$, any two connected graphs with isomorphic line graphs are isomorphic. It is an interesting exercise to show that the line graph of an Eulerian graph is both Eulerian and Hamiltonian, while the line graph of a Hamiltonian graph is always Hamiltonian.

Related Problems: Vertex coloring (see page 544), scheduling (see page 468).





INPUT OUTPUT

16.9 Graph Isomorphism

Input description: Two graphs, G and H.

Problem description: Find a (or all) mapping f from the vertices of G to the vertices of H such that G and H are identical; i.e. , (x, y) is an edge of G iff $(f(x), f(y))$ is an edge of H.

Discussion: Isomorphism is the problem of testing whether two graphs are really the same. Suppose we are given a collection of graphs and must perform some operation on each of them. If we can identify which of the graphs are duplicates, we can discard copies to avoid redundant work.

Certain pattern recognition problems are readily mapped to graph or subgraph isomorphism detection. The structure of chemical compounds are naturally described by labeled graphs, with each atom represented by a vertex. Identifying all molecules in a structure database containing a particular functional group is an instance of subgraph isomorphism testing.

We need some terminology to settle what is meant when we say two graphs are the same. Two labeled graphs $G = (V_g, E_g)$ and $H = (V_h, E_h)$ are *identical* when $(x, y) \in E_g$ iff $(x, y) \in E_h$. The isomorphism problem consists of finding a mapping from the vertices of G to H such that they are identical. Such a mapping is called an *isomorphism*; the problem of finding the mapping is sometimes called *graph matching*.

Identifying symmetries is another important application of graph isomorphism. A mapping of a graph to itself is called an *automorphism*, and the collection of

automorphisms (the automorphism *group*) provides a great deal of information about symmetries in the graph. For example, the complete graph K_n has $n!$ automorphisms (any mapping will do), while an arbitrary random graph is likely to have few or perhaps only one, since G is always identical to itself.

Several variations of graph isomorphism arise in practice:

- *Is graph G contained in graph H?* – Instead of testing equality, we are often interested in knowing whether a small pattern graph G is a *subgraph* of H. Such problems as clique, independent set, and Hamiltonian cycle are important special cases of subgraph isomorphism.

  There are two distinct graph-theoretic notions of "contained in." *Subgraph isomorphism* asks whether there is a subset of edges and vertices of H that is isomorphic to a smaller graph G. *Induced subgraph isomorphism* asks whether there is a subset of vertices of H whose deletion leaves a subgraph isomorphic to a smaller graph G. For induced subgraph isomorphism, (1) all edges of G must be present in H, and (2) no *non-edges* of G can be present in H. Clique happens to be an instance of both subgraph isomorphism problems, while Hamiltonian cycle is only an example of vanilla subgraph isomorphism.

  Be aware of this distinction in your application. Subgraph isomorphism problems tend to be harder than graph isomorphism, while induced subgraph problems tend to be even harder than subgraph isomorphism. Some flavor of backtracking is your only viable approach.

- *Are your graphs labeled or unlabeled?* – In many applications, vertices or edges of the graphs are *labeled* with some attribute that must be respected in determining isomorphisms. For example, in comparing two bipartite graphs, each with "worker" vertices and "job" vertices, any isomorphism that equated a job with a worker would make no sense.

  Labels and related constraints can be factored into any backtracking algorithm. Further, such constraints significantly speed up the search, by creating many more opportunities for pruning whenever two vertex labels do not match up.

- *Are you testing whether two trees are isomorphic?* – Faster algorithms exist for certain special cases of graph isomorphism, such as trees and planar graphs. Perhaps the most important case is detecting isomorphisms among trees, a problem that arises in language pattern matching and parsing applications. A parse tree is often used to describe the structure of a text; two parse trees will be isomorphic if the underlying pair of texts have the same structure.

  Efficient algorithms for tree isomorphism begin with the leaves of both trees and work inward toward the center. Each vertex in one tree is assigned a label representing the set of vertices in the second tree that might possibly

be isomorphic to it, based on the constraints of labels and vertex degrees. For example, all the leaves in tree T_1 are initially potentially equivalent to all leaves of T_2. Now, working inward, we can partition the vertices adjacent to leaves in T_1 into classes based on how many leaves and non-leaves they are adjacent to. By carefully keeping track of the labels of the subtrees, we can make sure that we have the same distribution of labeled subtrees for T_1 and T_2. Any mismatch means $T_1 \neq T_2$, while completing the process partitions the vertices into equivalence classes defining all isomorphisms. See the references below for more details.

- *How many graphs do you have?* – Many data mining applications involve searching for all instances of a particular pattern graph in a big database of graphs. The chemical structure mapping application described above falls into this family. Such databases typically contain a large number of relatively small graphs. This puts an onus on indexing the graph database by small substructures (say five to ten vertex each), and doing expensive isomorphism tests only against those containing the same substructures as the query graph.

No polynomial-time algorithm is known for graph isomorphism, but neither is it known to be NP-complete. Along with integer factorization (see Section 13.8 (page 420)), it is one of the few important algorithmic problems whose rough computational complexity is still not known. The conventional wisdom is that isomorphism is a problem that lies between P and NP-complete if P $\neq$ NP.

Although no worst-case polynomial-time algorithm is known, testing isomorphism is *usually* not very hard in practice. The basic algorithm backtracks through all $n!$ possible relabelings of the vertices of graph h with the names of vertices of graph g, and then tests whether the graphs are identical. Of course, we can prune the search of all permutations with a given prefix as soon as we detect any mismatch between edges whose vertices are both in the prefix.

However, the real key to efficient isomorphism testing is to preprocess the vertices into "equivalence classes," partitioning them into sets of vertices so that two vertices in different sets cannot possibly be mistaken for each other. All vertices in each equivalence class must share the same value of some invariant that is independent of labeling. Possibilities include:

- *Vertex degree* – This simplest way to partition vertices is based on their degree—the number of edges incident on the vertex. Two vertices of different degrees cannot be identical. This simple partition can be a big win, but won't do much for regular (equal degree) graphs.

- *Shortest path matrix* – For each vertex v, the all-pairs shortest path matrix (see Section 15.4 (page 489)) defines a multiset of $n-1$ distances representing the distances between v and each of the other vertices. Any two identical vertices must define the exact same multiset of distances, so we can partition the vertices into equivalence classes defining identical distance multisets.

- *Counting length-k paths* – Taking the adjacency matrix of G and raising it to the kth power gives a matrix where $G^k[i,j]$ counts the number of (nonsimple) paths from i to j. For each vertex and each k, this matrix defines a multiset of path-counts, which can be used for partitioning as with distances above. You could try all $1 \leq k \leq n$ or beyond, and use any single deviation as an excuse to partition.

Using these invariants, you should be able to partition the vertices of most graphs into a large number of small equivalence classes. Finishing the job off with backtracking should then be short work. We assign each vertex the name of its equivalence class as a label, and treat it as a labeled matching problem. It is harder to detect isomorphisms between highly-symmetric graphs than it is with random graphs because of the reduced effectiveness of these equivalence-class partitioning heuristics.

Implementations: The best known isomorphism testing program is `nauty` (No AUTomorphisms, Yes?)—a set of very efficient C language procedures for determining the automorphism group of a vertex-colored graph. Nauty is also able to produce a canonically-labeled isomorph of the graph, to assist in isomorphism testing. It was the basis of the first program to generate all 11-vertex graphs without isomorphs, and can test most graphs with fewer than 100 vertices in well under a second. Nauty has been ported to a variety of operating systems and C compilers. It is available at *http://cs.anu.edu.au/∼bdm/nauty/*. The theory behind `nauty` is described in [McK81].

The `VFLib` graph-matching library contains implementations for several different algorithms for *both* graph and subgraph isomorphism testing. This library has been widely used and very carefully benchmarked [FSV01]. It is available at *http://amalfi.dis.unina.it/graph/*.

`GraphGrep` [GS02] (*http://www.cs.nyu.edu/shasha/papers/graphgrep/*) is a representative data mining tool for querying large databases of graphs.

Valiente [Val02] has made available the implementations of graph/subgraph isomorphism algorithms for both trees and graphs in his book [Val02]. These C++ implementations run on top of LEDA (see Section 19.1.1 (page 658)), and are available at *http://www.lsi.upc.edu/∼valiente/algorithm/*.

Kreher and Stinson [KS99] compute isomorphisms of graphs in addition to more general group-theoretic operations. These implementations in C are available at *http://www.math.mtu.edu/∼kreher/cages/Src.html*.

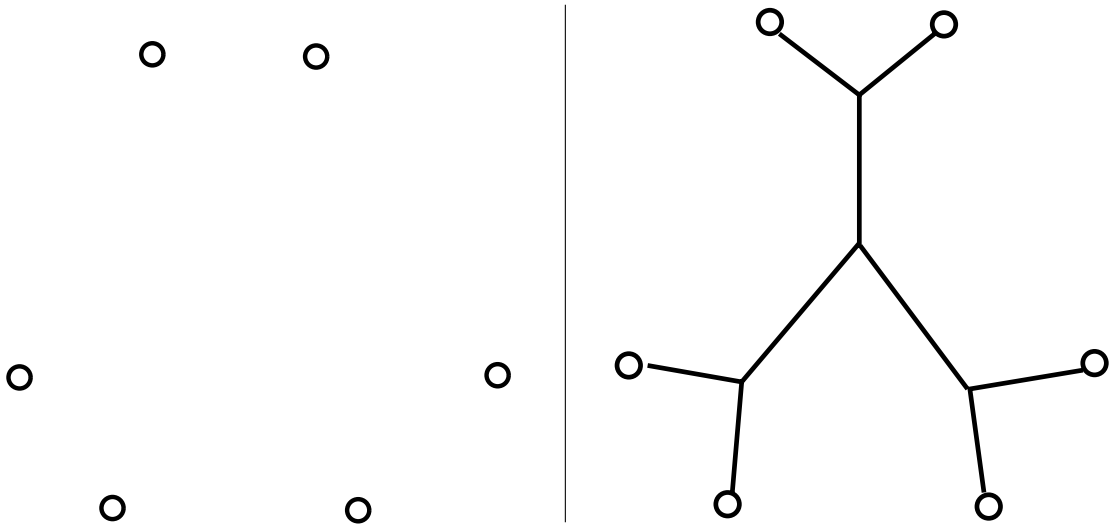
Notes: Graph isomorphism is an important problem in complexity theory. Monographs on isomorphism detection include [Hof82, KST93]. Valiente [Val02] focuses on algorithms for tree and subgraph isomorphism. Kreher and Stinson [KS99] take a more group-theoretic approach to isomorphism testing. Graph mining systems and algorithms are surveyed in [CH06]. See [FSV01] for performance comparisons between different graph and subgraph isomorphism algorithms.

Polynomial-time algorithms are known for planar graph isomorphism [HW74] and for graphs where the maximum vertex degree is bounded by a constant [Luk80]. The all-pairs

shortest path heuristic is due to [SD76], although there exist nonisomorphic graphs that realize the exact same set of distances [BH90]. A linear-time tree isomorphism algorithm for both labeled and unlabeled trees is presented in [AHU74].

A problem is said to be *isomorphism-complete* if it is provably as hard as isomorphism. Testing the isomorphism of bipartite graphs is isomorphism-complete, since any graph can be made bipartite by replacing each edge by two edges connected with a new vertex. Clearly, the original graphs are isomorphic if and only if the transformed graphs are.

Related Problems: Shortest path (see page 489), string matching (see page 628).



INPUT OUTPUT

16.10 Steiner Tree

Input description: A graph $G = (V, E)$. A subset of vertices $T \in V$.

Problem description: Find the smallest tree connecting all the vertices of T.

Discussion: Steiner trees arise often in network design problems, since the minimum Steiner tree describes how to connect a given set of sites using the smallest amount of wire. Analogous problems occur when designing networks of water pipes or heating ducts and in VLSI circuit design. Typical Steiner tree problems in VLSI are to connect a set of sites to (say) ground under constraints such as material cost, signal propagation time, or reducing capacitance.

The Steiner tree problem is distinguished from the minimum spanning tree (MST) problem (see Section 15.3 (page 484)) in that we are permitted to construct or select intermediate connection points to reduce the cost of the tree. Issues in Steiner tree construction include:

- *How many points do you have to connect?* – The Steiner tree of a pair of vertices is simply the shortest path between them (see Section 15.4 (page 489)). The Steiner tree of all the vertices, when $S = V$, simply defines the MST of G. The general minimum Steiner tree problem is NP-hard despite these special cases, and remains so under a broad range of restrictions.

- *Is the input a set of geometric points or a distance graph?* – Geometric versions of Steiner tree take a set of points as input, typically in the plane, and seek the smallest tree connecting the points. A complication is that the set of possible intermediate points is not given as part of the input but must be deduced from the set of points. These possible Steiner points must satisfy several geometric properties, which can be used to reduce the set of candidates down to a finite number. For example, every Steiner point will have a degree of exactly three in a minimum Steiner tree, and the angles formed between any two of these edges must be exactly 120 degrees.

- *Are there constraints on the edges we can use?* – Many wiring problems correspond to geometric versions of the problem, where all edges are restricted to being either horizontal or vertical. This is the so-called *rectilinear Steiner problem*. A different set of angular and degree conditions apply for rectilinear Steiner trees than for Euclidean trees. In particular, all angles must be multiples of 90 degrees, and each vertex is of a degree up to four.

- *Do I really need an optimal tree?* – Certain Steiner tree applications (e.g., circuit design and communications networks) justify investing large amounts of computation to find the best possible Steiner tree. This implies an exhaustive search technique such as backtracking or branch-and-bound. There are many opportunities for pruning search based on geometric and graph-theoretic constraints.

  Still, Steiner tree remains a hard problem. We recommend experimenting with the implementations described below before attempting your own.

- *How can I reconstruct Steiner vertices I never knew about?* – A very special type of Steiner tree arises in classification and evolution. A *phylogenic tree* illustrates the relative similarity between different objects or species. Each object represents (typically) a leaf/terminal vertex of the tree, with intermediate vertices representing branching points between classes of objects. For example, an evolutionary tree of animal species might have leaf nodes of *human, dog, snake* and internal nodes corresponding to taxa *(animal, mammal, reptile)*. A tree rooted at *animal* with *dog* and *human* classified under *mammal* implies that humans are closer to dogs than to snakes.

  Many different phylogenic tree construction algorithms have been developed that vary in (1) the data they attempt to model, and (2) the desired optimization criterion. Each combination of reconstruction algorithm and distance measure is likely to give a different answer, so identifying the "right" method for any given application is somewhat a question of faith. A reasonable procedure is to acquire a standard package of implementations, discussed below, and then see what happens to your data under all of them.

Fortunately, there is a good, efficient heuristic for finding Steiner trees that works well on all versions of the problem. Construct a graph modeling your input,

setting the weight of edge (i, j) equal to the distance from point i to point j. Find an MST of this graph. You are guaranteed a provably good approximation for both Euclidean and rectilinear Steiner trees.

The worst case for a MST approximation of the Euclidean Steiner tree is three points forming an equilateral triangle. The MST will contain two of the sides (for a length of 2), whereas the minimum Steiner tree will connect the three points using an interior point, for a total length of $\sqrt{3}$. This ratio of $\sqrt{3}/2 \approx 0.866$ is always achieved, and in practice the easily-computed MST is usually within a few percent of the optimal Steiner tree. The rectilinear Steiner tree / MST ratio is always $\geq 2/3 \approx 0.667$.

Such an MST can be refined by inserting a Steiner point whenever the edges of the minimum spanning tree incident on a vertex form an angle of less than 120 degrees between them. Inserting these points and locally readjusting the tree edges can move the solution a few more percent towards the optimum. Similar optimizations are possible for rectilinear spanning trees.

Note that we are only interested in the subtree connecting the terminal vertices. We may need to trim the MST if we add nonterminal vertices to the input of the problem. We retain only the tree edges which lie on the (unique) path between some pair of terminal nodes. The complete set of these can be found in $O(n)$ time by performing a BFS on the full tree starting from any single terminal node.

An alternative heuristic for graphs is based on shortest path. Start with a tree consisting of the shortest path between two terminals. For each remaining terminal t, find the shortest path to a vertex v in the tree and add this path to the tree. The time complexity and quality of this heuristic depend upon the insertion order of the terminals and how the shortest-path computations are performed, but something simple and fairly effective is likely to result.

Implementations: GeoSteiner is a package for solving both Euclidean and rectilinear Steiner tree problems in the plane by Warme, Winter, and Zachariasen [WWZ00]. It also solves the related problem of MSTs in hypergraphs, and claims to have solved problems as large as 10,000 points to optimality. It is available from *http://www.diku.dk/geosteiner/*. This is almost certainly the best code for geometric instances of Steiner tree.

FLUTE (*http://home.eng.iastate.edu/~cnchu/flute.html*) computes rectilinear Steiner trees, emphasizing speed. It contains a user-defined parameter to control the tradeoff between solution quality and run time.

GOBLIN (*http://www.math.uni-augsburg.de/~fremuth/goblin.html*) includes both heuristics and search methods for finding Steiner trees in graphs.

The programs PHYLIP (*http://evolution.genetics.washington.edu/phylip.html*) and PAUP (*http://paup.csit.fsu.edu/*) are widely-used packages for inferring phylogenic trees. Both contain over 20 different algorithms for constructing phylogenic trees from data. Although many of them are designed to work with molecular sequence data, several general methods accept arbitrary distance matrices as input.

Notes: Recent monographs on the Steiner tree problem include Hwang, Richards, and Winter [HRW92] and Prömel and Steger [PS02]. Du, et al. [DSR00] is a collection of recent surveys on all aspects of Steiner trees. Older surveys on the problem include [Kuh75]. Empirical results on Steiner tree heuristics include [SFG82, Vos92].

The Euclidean Steiner problem dates back to Fermat, who asked how to find a point p in the plane minimizing the sum of the distances to three given points. This was solved by Torricelli before 1640. Steiner was apparently one of several mathematicians who worked the general problem for n points, and was mistakenly credited with the problem. An interesting, more detailed history appears in [HRW92].

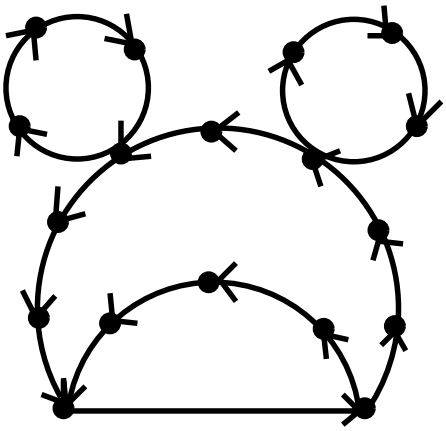
Gilbert and Pollak [GP68] first conjectured that the ratio of the length of the minimum Steiner tree over the MST is always $\geq \sqrt{3}/2 \approx 0.866$. After twenty years of active research, the Gilbert-Pollak ratio was finally proven by Du and Hwang [DH92]. The Euclidean MST for n points in the plane can be constructed in $O(n \lg n)$ time [PS85].

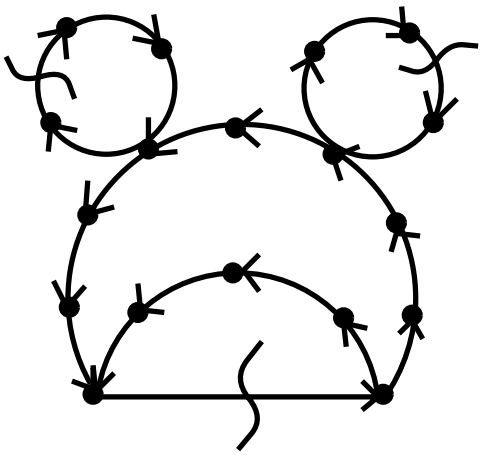
Arora [Aro98] gave a polynomial-time approximation scheme (PTAS) for Steiner trees in k-dimensional Euclidian space. A 1.55-factor approximation for Steiner trees on graphs is due to Robins and Zelikovsky [RZ05].

Expositions on the proof that the Steiner tree problem for graphs is hard [Kar72] include [Eve79a]. Expositions on exact algorithms for Steiner trees in graphs include [Law76]. The hardness of Steiner tree for Euclidean and rectilinear metrics was established in [GGJ77, GJ77]. Euclidean Steiner tree is not known to be in NP, because of numerical issues in representing distances.

Analogies can be drawn between minimum Steiner trees and minimum energy configurations in certain physical systems. The case that such analog systems—including the behavior of soap films over wire frames—"solve" the Steiner tree problem is discussed in [Mie58].

Related Problems: Minimum spanning tree (see page 484), shortest path (see page 489).





INPUT OUTPUT

16.11 Feedback Edge/Vertex Set

Input description: A (directed) graph $G = (V, E)$.

Problem description: What is the smallest set of edges E' or vertices V' whose deletion leaves an acyclic graph?

Discussion: Feedback set problems arise because many things are easier to do on directed acyclic graphs (DAGs) than general digraphs. Consider the problem of scheduling jobs with precedence constraints (i.e. , job A must come before job B). When the constraints are all consistent, the resulting graph is a DAG, and topological sort (see Section 15.2 (page 481)) can be used to order the vertices to respect them. But how can you design a schedule when there are cyclic constraints, such as A must be done before B, which must be done before C, which must be done before A?

By identifying a feedback set, we identify the smallest number of constraints that must be dropped to permit a valid schedule. In the *feedback edge* (or arc) set problem, we drop individual precedence constraints. In the *feedback vertex set* problem, we drop entire jobs and all constraints associated with them.

Similar considerations are involved in eliminating race conditions from electronic circuits. This explains why the problem is called "feedback" set. It is also known as the *maximum acyclic subgraph problem.*

One final application has to do with ranking tournaments. Suppose we want to rank order the skills of players at some two-player game, such as chess or tennis. We can construct a directed graph where there is an arc from x to y if x beats y in a game. The higher-ranked player *should* be at the lower-ranked player, although upsets often occur. A natural ranking is the topological sort resulting after deleting the minimum set of feedback edges (upsets) from the graph.

Issues in feedback set problems include:

- *Do* any *constraints have to be dropped?* – No changes are needed if the graph is already a DAG, which can be determined via topological sort. One way to find a feedback set modifies the topological sorting algorithm to delete whatever edge or vertex is causing the trouble whenever a contradiction is found. This feedback set might be much larger than needed, however, since feedback edge set and feedback vertex set are NP-complete on directed graphs.

- *How can I find a good feedback edge set?* – An effective linear-time heuristic constructs a vertex ordering and then deletes any arc going in the wrong direction. At least half the arcs must go either left-to-right or right-to-left for any vertex order, so take the smaller partition as your feedback set.

  But what is the right vertex order to start from? One natural order is to sort the vertices in terms of edge-imbalance, namely in-degree minus out-degree. Another approach starts by picking an arbitrary vertex v. Any vertex x defined by an in-going edge (x, v) will be placed to the left of v. Any x defined by out-going edge (v, x) will analogously be placed to the right of v. We can now recur on the left and right subsets to complete the vertex order.

- *How can I find a good feedback vertex set?* – The heuristics above yield vertex orders defining (hopefully) few back edges. We seek a small set of vertices that together cover these backedges. This is exactly a vertex cover problem, the heuristics for which are discussed in Section 16.3 (page 530).

- *What if I want to break all cycles in an undirected graph?* – The problem of finding feedback sets in undirected graphs is quite different from digraphs. Trees are undirected graphs without cycles, and every tree on n vertices contains exactly $n - 1$ edges. Thus the smallest feedback edge set of any undirected graph G is $|E| - (n - c)$, where c is the number of connected components of G. The back edges encountered during a depth-first search of G qualified as a minimum feedback edge set.

  The feedback vertex set problem remains NP-complete for undirected graphs, however. A reasonable heuristic uses breadth-first search to identify the shortest cycle in G. The vertices in this cycle are all deleted from G, and the shortest remaining cycle identified. This find-and-delete procedure is employed until the graph is acyclic. The optimal feedback vertex set must contain at least one vertex from each of these vertex-disjoint cycles, so the average deleted-cycle length determines just how good our approximation is.

It may pay to refine any of these heuristic solutions using randomization or simulated annealing. To move between states, we can modify the vertex permutation by swapping pairs in order or insert/delete vertices to/from the candidate feedback set.

Implementations: Greedy randomized adaptive search (GRASP) heuristics for both feedback vertex and feedback edge set problems have been implemented by Festa, et al. [FPR01] as Algorithm 815 of the *Collected Algorithms of the ACM* (see Section 19.1.6 (page 659)). These Fortran codes are also available from *http://www.research.att.com/∼mgcr/src/*.

GOBLIN (*http://www.math.uni-augsburg.de/∼fremuth/goblin.html*) includes an approximation heuristic for minimum feedback arc set.

The econ_order program of the Stanford GraphBase (see Section 19.1.8 (page 660)) permutes the rows and columns of a matrix so as to minimize the sum of the numbers below the main diagonal. Using an adjacency matrix as the input and deleting all edges below the main diagonal leaves an acyclic graph.

Notes: See [FPR99] for a survey on the feedback set problem. Expositions of the proofs that feedback minimization is hard [Kar72] include [AHU74, Eve79a]. Both feedback vertex and edge set remain hard even if no vertex has in-degree or out-degree greater than two [GJ79].

Bafna, et al. [BBF99] gives a 2-factor approximation for feedback vertex set in undirected graphs. Feedback edge sets in directed graphs can be approximated to within a factor of $O(\log n \log \log n)$ [ENSS98]. Heuristics for ranking tournaments are discussed in [CFR06]. Experiments with heuristics are reported in [Koe05].

An interesting application of feedback arc set to economics is presented in [Knu94]. For each pair A, B of sectors of the economy, we are given how much money flows from A to B. We seek to order the sectors to determine which sectors are primarily producers to other sectors, and which deliver primarily to consumers.

Related Problems: Bandwidth reduction (see page 398), topological sorting (see page 481), scheduling (see page 468).

17

Computational Geometry

Computational geometry is the algorithmic study of geometric problems. Its emergence coincided with application areas such as computer graphics, computer-aided design/manufacturing, and scientific computing, which together provide much of the motivation for geometric computing. The past twenty years have seen enormous maturity in computational geometry, resulting in a significant body of useful algorithms, software, textbooks, and research results.

Good books on computational geometry include:

- *de Berg, et al.* [dBvKOS00] – The "three Mark's" book is the best general introduction to the theory of computational geometry and its fundamental algorithms.

- *O'Rourke* [O'R01] – This is the best practical introduction to computational geometry. The emphasis is on careful and correct implementation of geometric algorithms. C and Java code are available from *http://maven.smith.edu/∼orourke/books/compgeom.html*.

- *Preparata and Shamos* [PS85] – Although somewhat out of date, this book remains a good general introduction to computational geometry, stressing algorithms for convex hulls, Voronoi diagrams, and intersection detection.

- *Goodman and O'Rourke* [GO04] – This recent collection of survey articles provides a detailed overview of what is known in most every subfield of discrete and computational geometry.

The leading conference in computational geometry is the *ACM Symposium on Computational Geometry*, held annually in late May or early June. Although the primary results presented at the conference are theoretical, there has been a

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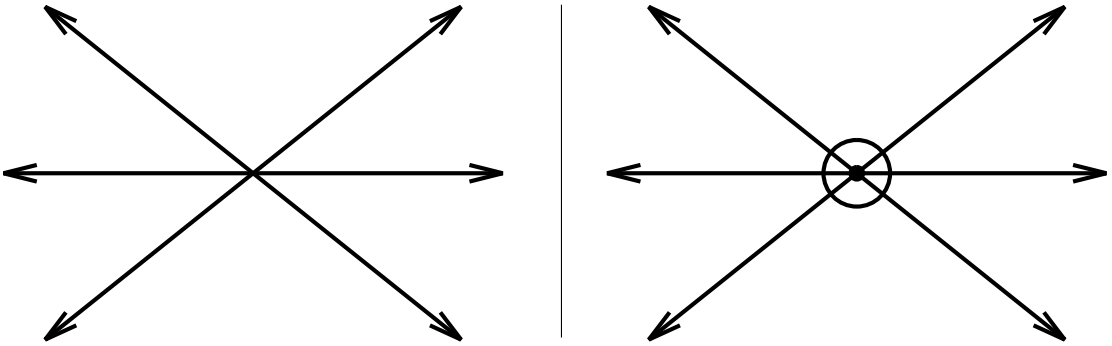
concerted effort on the part of the research community to increase the presence of applied, experimental work through video reviews and poster sessions.

There is a growing body of implementations of geometric algorithms. We point out specific implementations where applicable in the catalog, but the reader should be particularly aware of `CGAL` (Computational Geometry Algorithms Library)—a comprehensive library of geometric algorithms in C++ produced as a result of a joint European project. Anyone with a serious interest in geometric computing should check it out at *http://www.cgal.org/*.



INPUT OUTPUT

17.1 Robust Geometric Primitives

Input description: A point p and line segment l, or two line segments l_1, l_2.

Problem description: Does p lie over, under, or on l? Does l_1 intersect l_2?

Discussion: Implementing basic geometric primitives is a task fraught with peril, even for such simple tasks as returning the intersection point of two lines. It is more complicated than you may think. What should you return if the two lines are parallel, meaning they don't intersect at all? What if the lines are identical, so the intersection is not a point but the entire line? What if one of the lines is horizontal, so that in the course of solving the equations for the intersection point you are likely to divide by zero? What if the two lines are almost parallel, so that the intersection point is so far from the origin as to cause arithmetic overflows? These issues become even more complicated for intersecting line segments, since there are many other special cases that must be watched for and treated specially.

If you are new to implementing geometric algorithms, I suggest that you study O'Rourke's *Computational Geometry in C* [O'R01] for practical advice and complete implementations of basic geometric algorithms and data structures. You are likely to avoid many headaches by following in his footsteps.

There are two different issues at work here: geometric degeneracy and numerical stability. *Degeneracy* refers to annoying special cases that must be treated in substantially different ways, such as when two lines intersect in more or less than a single point. There are three primary approaches to dealing with degeneracy:

- *Ignore it* – Make as an operating assumption that your program will work correctly only if no three points are collinear, no three lines meet at a point, no intersections happen at the endpoints of line segments, etc. This is probably the most common approach, and what I might recommend for short-term

projects if you can live with frequent crashes. The drawback is that interesting data often comes from points sampled on a grid, and so is inherently very degenerate.

- *Fake it* – Randomly or symbolically perturb your data so that it becomes nondegenerate. By moving each of your points a small amount in a random direction, you can break many of the existing degeneracies in the data, hopefully without creating too many new problems. This probably should be the first thing to try once you decide that your program is crashing too often. A problem with random perturbations is that they can change the shape of your data in subtle ways, which may be intolerable for your application. There also exist techniques to "symbolically" perturb your data to remove degeneracies in a consistent manner, but these require serious study to apply correctly.
- *Deal with it* – Geometric applications can be made more robust by writing special code to handle each of the special cases that arise. This can work well if done with care at the beginning, but not so well if kludges are added whenever the system crashes. Expect to expend significant effort if you are determined to do it right.

Geometric computations often involve floating-point arithmetic, which leads to problems with overflows and numerical precision. There are three basic approaches to the issue of numerical stability:

- *Integer arithmetic* – By forcing all points of interest to lie on a fixed-size integer grid, you can perform exact comparisons to test whether any two points are equal or two line segments intersect. The cost is that the intersection point of two lines may not be exactly representable as a grid point. This is likely to be the simplest and best method, if you can get away with it.
- *Double precision reals* – By using double-precision floating point numbers, you may get lucky and avoid numerical errors. Your best bet might be to keep all the data as single-precision reals, and use double-precision for intermediate computations.
- *Arbitrary precision arithmetic* – This is certain to be correct, but also to be slow. This approach seems to be gaining favor in the research community. Careful analysis can minimize the need for high-precision arithmetic and thus the performance penalty. Still, you should expect high-precision arithmetic to be several orders of magnitude slower than standard floating-point arithmetic.

The difficulties associated with producing robust geometric software are still under attack by researchers. The best practical technique is to base your applications on a small set of geometric primitives that handle as much of the low-level geometry as possible. These primitives include:

- *Area of a triangle* – Although it is well known that the area $A(t)$ of a triangle $t = (a, b, c)$ is half the base times the height, computing the length of the base and altitude is messy work with trigonometric functions. It is better to use the determinant formula for *twice* the area:

$$2 \cdot A(t) = \begin{vmatrix} a_x & a_y & 1 \\ b_x & b_y & 1 \\ c_x & c_y & 1 \end{vmatrix} = a_x b_y - a_y b_x + a_y c_x - a_x c_y + b_x c_y - c_x b_y$$

  This formula generalizes to compute $d!$ times the volume of a simplex in d dimensions. Thus, $3! = 6$ times the volume of a tetrahedron $t = (a, b, c, d)$ in three dimensions is

$$6 \cdot A(t) = \begin{vmatrix} a_x & a_y & a_z & 1 \\ b_x & b_y & b_z & 1 \\ c_x & c_y & c_z & 1 \\ d_x & d_y & d_z & 1 \end{vmatrix}$$

  Note that these are signed volumes and can be negative, so take the absolute value first. Section 13.4 (page 404) explains how to compute determinants.

  The conceptually simplest way to compute the area of a polygon (or polyhedron) is to triangulate it and then sum up the area of each triangle. Implementations of a slicker algorithm that avoids triangulation are discussed in [O'R01, SR03].

- *Above-below-on test* – Does a given point c lie above, below, or on a given line l? A clean way to deal with this is to represent l as a directed line that passes through point a before point b, and ask whether c lies to the left or right of the directed line l. It is up to you to decide whether left means above or below.

  This primitive can be implemented using the sign of the triangle area as computed above. If the area of $t(a, b, c) > 0$, then c lies to the left of $\overline{ab}$. If the area of $t(a, b, c) = 0$, then c lies on $\overline{ab}$. Finally, if the area of $t(a, b, c) < 0$, then c lies to the right of $\overline{ab}$. This generalizes naturally to three dimensions, where the sign of the area denotes whether d lies above or below the oriented plane (a, b, c).

- *Line segment intersection* – The above-below primitive can be used to test whether a line intersects a line segment. It does iff one endpoint of the segment is to the left of the line and the other is to the right. Segment intersection is similar but more complicated. We refer you to implementations described below. The decision as to whether two segments intersect if they share an endpoint depends upon your application and is representative of the problems with degeneracy.

- *In-circle test* – Does point d lie inside or outside the circle defined by points a, b, and c in the plane? This primitive occurs in all Delaunay triangulation algorithms, and can be used as a robust way to do distance comparisons. Assuming that a, b, c are labeled in counterclockwise order around the circle, compute the determinant

$$\text{incircle}(a,b,c,d) = \begin{vmatrix} a_x & a_y & a_x^2+a_y^2 & 1 \\ b_x & b_y & b_x^2+b_y^2 & 1 \\ c_x & c_y & c_x^2+c_y^2 & 1 \\ d_x & d_y & d_x^2+d_y^2 & 1 \end{vmatrix}$$

  In-circle will return 0 if all four points are cocircular—a positive value if d is inside the circle, and negative if d is outside.

Check out the Implementations section before you build your own.

Implementations: CGAL (*www.cgal.org*) and LEDA (see Section 19.1.1 (page 658)) both provide very complete sets of geometric primitives for planar geometry written in C++. LEDA is easier to learn and to work with, but CGAL is more comprehensive and freely available. If you are starting a significant geometric application, you should at least check them out before you try to write your own.

O'Rourke [O'R01] provides implementations in C of most of the primitives discussed in this section. See Section 19.1.10 (page 662). These primitives were implemented primarily for exposition rather than production use, but they should be reliable and appropriate for small applications.

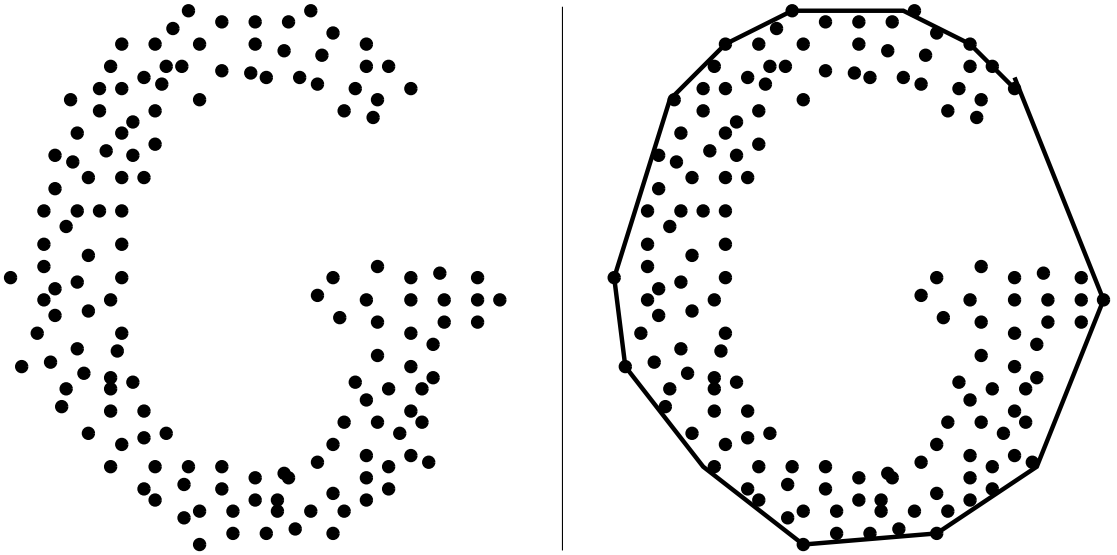
The *Core Library* (see *http://cs.nyu.edu/exact/*) provides an API, which supports the Exact Geometric Computation (EGC) approach to numerically robust algorithms. With small changes, any C/C++ program can use it to readily support three levels of accuracy: machine-precision, arbitrary-precision, and guaranteed.

Shewchuk's [She97] robust implementation of basic geometric primitives in C++ is available at *http://www.cs.cmu.edu/∼quake/robust.html*.

Notes: O'Rourke [O'R01] provides an implementation-oriented introduction to computational geometry which stresses robust geometric primitives. It is recommended reading. LEDA [MN99] provides another excellent role model.

Yap [Yap04] gives a excellent survey on techniques for achieving robust geometric computation, with a book [MY07] in preparation. Kettner, et al. [KMP+04] provides graphic evidence of the troubles that arise when employing real arithmetic in geometric algorithms such as convex hull. Controlled perturbation [MOS06] is a new approach for robust computation that is receiving considerable attention. Shewchuk [She97] and Fortune and van Wyk [FvW93] present careful studies on the costs of using arbitrary-precision arithmetic for geometric computation. By being careful about when to use it, reasonable efficiency can be maintained while achieving complete robustness.

Related Problems: Intersection detection (see page 591), maintaining arrangements (see page 614).



INPUT OUTPUT

17.2 Convex Hull

Input description: A set S of n points in d-dimensional space.

Problem description: Find the smallest convex polygon (or polyhedron) containing all the points of S.

Discussion: Finding the convex hull of a set of points is *the* most important elementary problem in computational geometry, just as sorting is the most important elementary problem in combinatorial algorithms. It arises because constructing the hull captures a rough idea of the shape or extent of a data set.

Convex hull serves as a first preprocessing step to many, if not most, geometric algorithms. For example, consider the problem of finding the diameter of a set of points, which is the pair of points that lie a maximum distance apart. The diameter must be between two points on the convex hull. The $O(n \lg n)$ algorithm for computing diameter proceeds by first constructing the convex hull, then for each hull vertex finding which other hull vertex lies farthest from it. The so-called "rotating-calipers" method can be used to move efficiently from one-diametrically opposed hull vertex to another by always proceeding in a clockwise fashion around the hull.

There are almost as many convex hull algorithms as sorting algorithms. Answer the following questions to help choose between them:

- *How many dimensions are you working with?* – Convex hulls in two and even three dimensions are fairly easy to work with. However, certain valid assumptions in lower dimensions break down as the dimensionality increases. For example, any n-vertex polygon in two dimensions has exactly n edges. However, the relationship between the numbers of faces and vertices becomes more complicated even in three dimensions. A cube has eight vertices and six faces, while an octahedron has eight faces and six vertices. This has implications for data structures that represent hulls—are you just looking for the hull points or do you need the defining polyhedron? Be aware of these complications of high-dimensional spaces if your problem takes you there.

  Simple $O(n \log n)$ convex-hull algorithms are available for the important special cases of two and three dimensions. In higher dimensions, things get more complicated. *Gift-wrapping* is the basic algorithm for constructing higher-dimensional convex hulls. Observe that a three-dimensional convex polyhedron is composed of two-dimensional faces, or *facets*, that are connected by one-dimensional lines or *edges*. Each edge joins exactly two facets together. Gift-wrapping starts by finding an initial facet associated with the lowest vertex and then conducting a breadth-first search from this facet to discover new, additional facets. Each edge e defining the boundary of a facet must be shared with one other facet. By running through each of the n points, we can identify which point defines the next facet with e. Essentially, we "wrap" the points one facet at a time by bending the wrapping paper around an edge until it hits the first point.

  The key to efficiency is making sure that each edge is explored only once. Implemented properly in d dimensions, gift-wrapping takes $O(n\phi_{d-1} + \phi_{d-2} \lg \phi_{d-2})$, where ϕ_{d-1} is the number of facets and ϕ_{d-2} is the number of edges in the convex hull. This can be as bad as $O(n^{\lfloor d/2 \rfloor + 1})$ when the convex hull is very complex. I recommend that you use one of the codes described below rather than roll your own.

- *Is your data given as vertices or half-spaces?* – The problem of finding the intersection of a set of n half-spaces in d dimensions (each containing the origin) is dual to that of computing convex hulls of n points in d dimensions. Thus, the same basic algorithm suffices for both problems. The necessary duality transformation is discussed in Section 17.15 (page 614). The problem of half-plane intersection differs from convex hull when no interior point is given, since the instance may be infeasible (i.e., the intersection of the half-planes empty).

- *How many points are likely to be on the hull?* – If your point set was generated "randomly," it is likely that most points lie within the interior of the hull. Planar convex-hull programs can be made more efficient in practice using the observation that the leftmost, rightmost, topmost, and bottommost points all must be on the convex hull. This usually gives a set of either three or

four distinct points, defining a triangle or quadrilateral. Any point inside this region *cannot* be on the convex hull and so can be discarded in a linear sweep through the points. Ideally, only a few points will then remain to run through the full convex-hull algorithm.

This trick can also be applied beyond two dimensions, although it loses effectiveness as the dimension increases.

- *How do I find the shape of my point set?* – Although convex hulls provide a gross measure of shape, any details associated with concavities are lost. The convex hull of the G from the example input would be indistinguishable from the convex hull of O. *Alpha-shapes* are a more general structure that can be parameterized so as to retain arbitrarily large concavities. Implementations and references on alpha-shapes are included below.

The primary convex-hull algorithm in the plane is the *Graham scan*. Graham scan starts with one point p known to be on the convex hull (say the point with the lowest x-coordinate) and sorts the rest of the points in angular order around p. Starting with a hull consisting of p and the point with the smallest angle, we proceed counterclockwise around v adding points. If the angle formed by the new point and the last hull edge is less than 180 degrees, we add this new point to the hull. If the angle formed by the new point and the last "hull" edge is greater than 180 degrees, then a chain of vertices starting from the last hull edge must be deleted to maintain convexity. The total time is $O(n \lg n)$, since the bottleneck is the cost of sorting the points around v.

The basic Graham scan procedure can also be used to construct a nonself-intersecting (or *simple*) polygon passing through all the points. Sort the points around v, but instead of testing angles, simply connect the points in angular order. Connecting this to v gives a polygon without self-intersection, although it typically has many ugly skinny protrusions.

The gift-wrapping algorithm becomes especially simple in two dimensions, since each "facet" becomes an edge, each "edge" becomes a vertex of the polygon, and the "breadth-first search" simply walks around the hull in a clockwise or counterclockwise order. The 2D gift-wrapping (or *Jarvis march*) algorithm runs in $O(nh)$ time, where h is the number of vertices on the convex hull. I recommend sticking with Graham scan unless you *really* know in advance that there cannot be too many vertices on the hull.

Implementations: The CGAL library (*www.cgal.org*) offers C++ implementations of an extensive variety of convex-hull algorithms for two, three, and arbitrary numbers of dimensions. Alternate C++ implementations of planar convex hulls includes LEDA (see Section 19.1.1 (page 658)).

Qhull [BDH97] is a popular low-dimensional, convex-hull code, optimized for from two to about eight dimensions. It is written in C and can also construct Delaunay triangulations, Voronoi vertices, furthest-site Voronoi vertices, and

half-space intersections. Qhull has been widely used in scientific applications and has a well-maintained homepage at *http://www.qhull.org/*.

O'Rourke [O'R01] provides a robust implementation of the Graham scan in two dimensions and an $O(n^2)$ implementation of an incremental algorithm for convex hulls in three dimensions. C and Java implementations are both available. See Section 19.1.10 (page 662).

For excellent alpha-shapes code, originating from the work of Edelsbrunner and Mucke [EM94], check out *http://biogeometry.duke.edu/software/alphashapes/*. Ken Clarkson's higher-dimensional convex-hull code *Hull* also does alpha-shapes, and is available at *http://www.netlib.org/voronoi/hull.html*.

Different codes are needed for enumerating the vertices of intersecting half-spaces in higher dimensions. Avis's *lhs* (*http://cgm.cs.mcgill.ca/~avis/C/lrs.html*) is an arithmetically-robust ANSI C implementation of the Avis-Fukuda reverse search algorithm for vertex enumeration/convex-hull problems. Since the polyhedra is implicitly traversed but not explicitly stored in memory, even problems with very large output sizes can sometimes be solved.

Notes: Planar convex hulls play a similar role in computational geometry as sorting does in algorithm theory. Like sorting, convex hull is a fundamental problem for which many different algorithmic approaches lead to interesting or optimal algorithms. Quickhull and mergehull are examples of hull algorithms inspired by sorting algorithms [PS85]. A simple construction involving points on a parabola presented in Section 9.2.4 (page 322) reduces sorting to convex hull, so the information-theoretic lower bound for sorting implies that planar convex hull requires $\Omega(n \lg n)$ time to compute. A stronger lower bound is established in [Yao81].

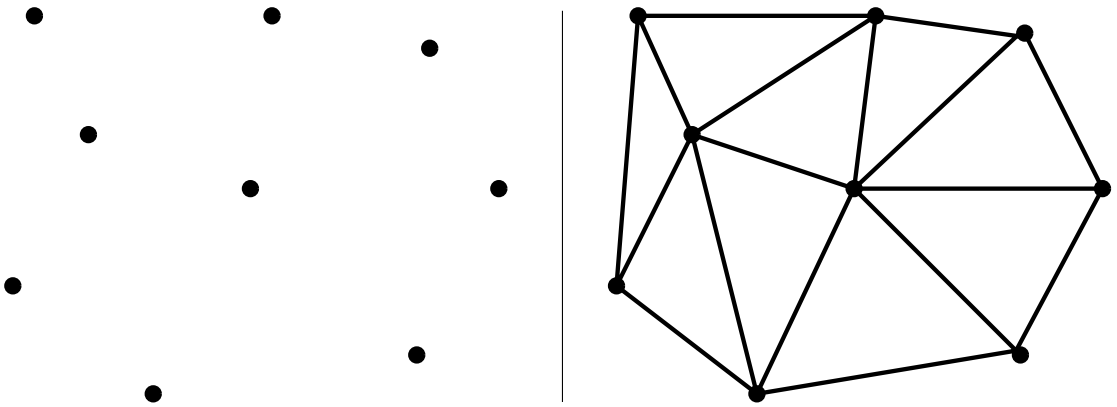
Good expositions of the Graham scan algorithm [Gra72] and the Jarvis march [Jar73] include [dBvKOS00, CLRS01, O'R01, PS85]. The optimal planar convex-hull algorithm [KS86] takes $O(n \lg h)$ time, where h is the number of hull vertices that captures the best performance of both Graham scan and gift wrapping and is (theoretically) better in between. Planar convex hull can be efficiently computed *in-place*, meaning without requiring additional memory in [BIK+04]. Seidel [Sei04] gives an up-to-date survey of convex hull algorithms and variants, particularly for higher dimensions.

Alpha-hulls, introduced in [EKS83], provide a useful notion of the shape of a point set. A generalization to three dimensions, with an implementation, is presented in [EM94].

Reverse-search algorithms for constructing convex hulls are effective in higher dimensions [AF96]. Through a clever lifting-map construction [ES86], the problem of building Voronoi diagrams in d-dimensions can be reduced to constructing convex hulls in $(d+1)$-dimensions. See Section 17.4 (page 576) for more details.

Dynamic algorithms for convex-hull maintenance are data structures that permit inserting and deleting arbitrary points while always representing the current convex hull. The first such dynamic data structure [OvL81] supported insertions and deletions in $O(\lg^2 n)$ time. More recently, Chan [Cha01] reduced the cost of such operation of near-logarithmic amortized time.

Related Problems: Sorting (see page 436), Voronoi diagrams (see page 576).



INPUT OUTPUT

17.3 Triangulation

Input description: A set of points or a polyhedron.

Problem description: Partition the interior of the point set or polyhedron into triangles.

Discussion: The first step in working with complicated geometric objects is often to break them into simple geometric objects. This makes triangulation a fundamental problem in computational geometry. The simplest geometric objects are triangles in two dimensions, and tetrahedra in three. Classical applications of triangulation include finite element analysis and computer graphics.

A particularly interesting application of triangulation is surface or function interpolation. Suppose that we have sampled the height of a mountain at a certain number of points. How can we estimate the height at any point q in the plane? We can project the sampled points on the plane, and then triangulate them. This triangulation partitions the plane into triangles, so we can estimate height by interpolating between the heights of the three points of the triangle that contain q. Furthermore, this triangulation and the associated height values define a mountain surface suitable for graphics rendering.

A triangulation in the plane is constructed by adding nonintersecting chords between the vertices until no more such chords can be added. Specific issues arising in triangulation include:

- *Are you triangulating a point set or a polygon?* – Often we are given a set of points to triangulate, as in the surface interpolation problem discussed

earlier. This involves first constructing the convex hull of the point set and then carving up the interior into triangles.

The simplest such $O(n \lg n)$ algorithm first sorts the points by x-coordinate. It then inserts them from left to right as per the convex-hull algorithm of page 105, building the triangulation by adding a chord to each point newly cut off from the hull.

- *Does the shape of the triangles in your triangulation matter?* – There are usually many different ways to partition your input into triangles. Consider a set of n points in convex position in the plane. The simplest way to triangulate them would be to add to the convex-hull diagonals from the first point to all of the others. However, this has the tendency to create skinny triangles.

  Many applications seek to to avoid skinny triangles, or equivalently, minimize small angles in the triangulation. The *Delaunay triangulation* of a point set minimizes the maximum angle over all possible triangulations. This isn't exactly what we are looking for, but it is pretty close, and the Delaunay triangulation has enough other interesting properties (including that it is dual to the Voronoi diagram) to make it the quality triangulation of choice. Further, it can be constructed in $O(n \lg n)$ time using implementations described below.

- *How can I improve the shape of a given triangulation?* – Each internal edge of any triangulation is shared between two triangles. The four vertices defining these two triangles form either (1) a convex quadrilateral, or (2) a triangle with a triangular bite taken out of it. The beauty of the convex case is that exchanging the internal edge with a chord linking the other two vertices yields a different triangulation.

  This gives us a local "edge-flip" operation for changing and possibly improving a given triangulation. Indeed, a Delaunay triangulation can be constructed from any initial triangulation by removing skinny triangles until no locally-improving exchange remains.

- *What dimension are we working in?* – Three-dimensional problems are usually harder than two-dimensional problems. The three-dimensional generalization of triangulation involves partitioning the space into four-vertex tetrahedra by adding nonintersecting faces. One important difficulty is that there is no way to tetrahedralize the interior of certain polyhedra without adding extra vertices. Furthermore, it is NP-complete to decide whether such a tetrahedralization exists, so we should not feel afraid to add extra vertices to simplify our problem.

- *What constraints does the input have?* – When we are triangulating a polygon or polyhedra, we are restricted to adding chords that do not intersect any of the boundary facets. In general, we may have a set of obstacles or

constraints that cannot be intersected by inserted chords. The best such triangulation is likely to be the so-called *constrained Delaunay triangulation*. Implementations are described next.

- *Are you allowed to add extra points, or move input vertices?* – When the shape of the triangles does matter, it might pay to strategically add a small number of extra "Steiner" points to the data set to facilitate the construction of a triangulation (say) with no small angles. As discussed above, *no* triangulation may exist for certain polyhedra without adding Steiner points.

To construct a triangulation of a convex polygon in linear time, just pick an arbitrary starting vertex v and insert chords from v to each other vertex in the polygon. Because the polygon is convex, we can be confident that none of the boundary edges of the polygon will be intersected by these chords, and that all of them lie within the polygon. The simplest algorithm for constructing general polygon triangulations tries each of the $O(n^2)$ possible chords and inserts them if they do not intersect a boundary edge or previously inserted chord. There are practical algorithms that run in $O(n \lg n)$ time and theoretically interesting algorithms that run in linear time. See the Implementations and Notes section for details.

Implementations: Triangle, by Jonathan Shewchuk, is an award-winning C language code that generates Delaunay triangulations, constrained Delaunay triangulations (forced to have certain edges), and quality-conforming Delaunay triangulations (which avoid small angles by inserting extra points). It has been widely used for finite element analysis and is fast and robust. Triangle is the first thing I would try if I needed a two-dimensional triangulation code. It is available at *http://www.cs.cmu.edu/~quake/triangle.html*.

Fortune's Sweep2 is a widely used 2D code for Voronoi diagrams and Delaunay triangulations, written in C. This code may be simpler to work with if all you need is the Delaunay triangulation of points in the plane. It is based on his sweepline algorithm [For87] for Voronoi diagrams and is available from Netlib (see Section 19.1.5 (page 659)) at *http://www.netlib.org/voronoi/*.

Mesh generation for finite element methods is an enormous field. Steve Owen's Meshing Research Corner (*http://www.andrew.cmu.edu/user/sowen/mesh.html*) provides a comprehensive overview of the literature, with links to an enormous variety of software. QMG (*http://www.cs.cornell.edu/Info/People/vavasis/qmg-home.html*) is a particularly recommended code.

Both the CGAL (*www.cgal.org*) and LEDA (see Section 19.1.1 (page 658)) libraries offer C++ implementations of an extensive variety of triangulation algorithms for two and three dimensions, including constrained and furthest site Delaunay triangulations.

Higher-dimensional Delaunay triangulations are a special case of higher-dimensional convex hulls. Qhull [BDH97] is a popular low-dimensional convex hull code, say for from two to about eight dimensions. It is written in C and can also construct Delaunay triangulations, Voronoi vertices, furthest-site Voronoi

vertices, and half-space intersections. Qhull has been widely used in scientific applications and has a well-maintained homepage at *http://www.qhull.org/*. Another choice is Ken Clarkson's higher-dimensional convex-hull code, *Hull*, available at *http://www.netlib.org/voronoi/hull.html*.

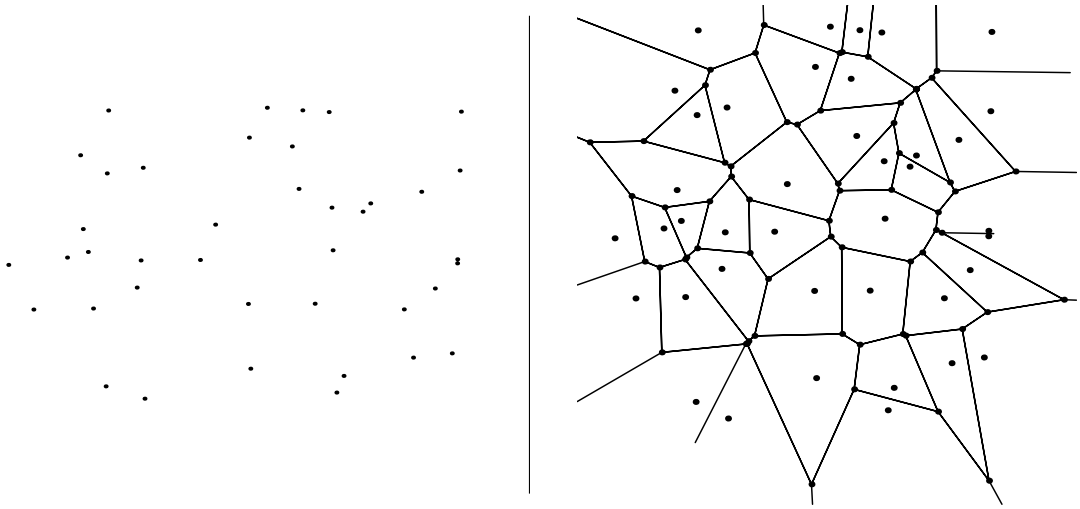
Notes: After a long search, Chazelle [Cha91] discovered a linear-time algorithm for triangulating a simple polygon. This algorithm is sufficiently hopeless to implement that it qualifies more as an existence proof. The first $O(n \lg n)$ algorithm for polygon triangulation was given by [GJPT78]. An $O(n \lg \lg n)$ algorithm by Tarjan and Van Wyk [TW88] followed before Chazelle's result. Bern [Ber04a] gives a recent survey on polygon and point-set triangulation.

The *International Meshing Roundtable* is an annual conference for people interested in mesh and grid generation. Excellent surveys on mesh generation include [Ber02, Ede06].

Linear-time algorithms for triangulating monotone polygons have been long known [GJPT78], and are the basis of algorithms for triangulating simple polygons. A polygon is monotone when there exists a direction d such that any line with slope d intersects the polygon in at most two points.

A heavily studied class of optimal triangulations seeks to minimize the total length of the chords used. The computational complexity of constructing this *minimum weight triangulation* was resolved when Rote [MR06] proved it NP-complete. Thus interest has shifted to provably good approximation algorithms. The minimum weight triangulation of a convex polygon can be found in $O(n^3)$ time using dynamic programming, as discussed in Section 8.6.1 (page 300).

Related Problems: Voronoi diagrams (see page 576), polygon partitioning (see page 601).



INPUT OUTPUT

17.4 Voronoi Diagrams

Input description: A set S of points $p_1, \ldots, p_n$.

Problem description: Decompose space into regions around each point such that all points in the region around p_i are closer to p_i than any other point in S.

Discussion: Voronoi diagrams represent the region of influence around each of a given set of sites. If these sites represent the locations of McDonald's restaurants, the Voronoi diagram partitions space into cells around each restaurant. For each person living in a particular cell, the defining McDonald's represents the closest place to get a Big Mac.

Voronoi diagrams have a surprising variety of applications:

- *Nearest neighbor search* – Finding the nearest neighbor of query point q from among a fixed set of points S is simply a matter of determining the cell in the Voronoi diagram of S that contains q. See Section 17.5 (page 580) for more details.

- *Facility location* – Suppose McDonald's wants to open another restaurant. To minimize interference with existing McDonald's, it should be located as far away from the closest restaurant as possible. This location is always at a vertex of the Voronoi diagram, and can be found in a linear-time search through all the Voronoi vertices.

- *Largest empty circle* – Suppose you needed to obtain a large, contiguous, undeveloped piece of land on which to build a factory. The same condition used to select McDonald's locations is appropriate for other undesirable facilities, namely that they be as far as possible from any relevant sites of interest. A Voronoi vertex defines the center of the largest empty circle among the points.

- *Path planning* – If the sites of S are the centers of obstacles we seek to avoid, the edges of the Voronoi diagram define the possible channels that maximize the distance to the obstacles. Thus the "safest" path among the obstacles will stick to the edges of the Voronoi diagram.

- *Quality triangulations* – In triangulating a set of points, we often desire nice, fat triangles that avoid small angles and skinny triangles. The *Delaunay triangulation* maximizes the minimum angle over all triangulations. Furthermore, it is easily constructed as the dual of the Voronoi diagram. See Section 17.3 (page 572) for details.

Each edge of a Voronoi diagram is a segment of the perpendicular bisector of two points in S, since this is the line that partitions the plane between the points. The conceptually simplest method to construct Voronoi diagrams is randomized incremental construction. To add another site to the diagram, we locate the cell that contains it and add the perpendicular bisectors separating this new site from all sites defining impacted regions. If the sites are inserted in random order, only a small number of regions are likely to be impacted with each insertion.

However, the method of choice is Fortune's sweepline algorithm, especially since robust implementations of it are readily available. The algorithm works by projecting the set of sites in the plane into a set of cones in three dimensions such that the Voronoi diagram is defined by projecting the cones back onto the plane. Advantages of Fortune's algorithm include that (1) it runs in optimal $\Theta(n \log n)$ time, (2) it is reasonable to implement, and (3) we need not store the entire diagram if we can use it as we sweep over it.

There is an interesting relationship between convex hulls in $d+1$ dimensions and Delaunay triangulations (or equivalently Voronoi diagrams) in d-dimensions. By projecting each site in E^d $(x_1, x_2, \ldots, x_d)$ into the point $(x_1, x_2, \ldots, x_d, \sum_{i=1}^{d} x_i^2)$, taking the convex hull of this $(d+1)$-dimensional point set and then projecting back into d dimensions, we obtain the Delaunay triangulation. Details are given in the Notes section, but this provides the best way to construct Voronoi diagrams in higher dimensions. Programs that compute higher-dimensional convex hulls are discussed in Section 17.2 (page 568).

Several important variations of standard Voronoi diagrams arise in practice. See the references below for details:

- *Non-Euclidean distance metrics* – Recall that Voronoi diagrams decompose space into regions of influence around each of the given sites. We have assumed that Euclidean distance measures influence, but this is inappropriate

for certain applications. If people drive to McDonald's, the time it takes to get there depends upon where the major roads are. Efficient algorithms are known for constructing Voronoi diagrams under a variety of different metrics, and for curved or constrained objects.

- *Power diagrams* – These structures decompose space into regions of influence around the sites, where the sites are no longer constrained to have all the same power. Imagine a map of radio stations operating at a given frequency. The region of influence around a station depends both on the power of its transmitter and the position/power of neighboring transmitters.

- *Kth-order and furthest-site diagrams* – The idea of decomposing space into regions sharing some property can be taken beyond closest-point Voronoi diagrams. Any point within a single cell of the kth-order Voronoi diagram shares the same set of k's closest points in S. In furthest-site diagrams, any point within a particular region shares the same furthest point in S. Point location (see Section 17.7 (page 587)) on these structures permits fast retrieval of the appropriate points.

Implementations: Fortune's Sweep2 is a widely used 2D code for Voronoi diagrams and Delaunay triangulations, written in C. This code is simple to work with if all you need is the Voronoi diagram. It is based on his sweepline algorithm [For87] for Voronoi diagrams and is available from Netlib (see Section 19.1.5 (page 659)) at *http://www.netlib.org/voronoi/*.

Both the CGAL (*www.cgal.org*) and LEDA (see Section 19.1.1 (page 658)) libraries offer C++ implementations of a variety of Voronoi diagram and Delaunay triangulation algorithms in two and three dimensions.

Higher-dimensional and furthest-site Voronoi diagrams can be constructed as a special case of higher-dimensional convex hulls. Qhull [BDH97] is a popular low-dimensional convex-hull code, useful for from two to about eight dimensions. It is written in C and can also construct Delaunay triangulations, Voronoi vertices, furthest-site Voronoi vertices, and half-space intersections. Qhull has been widely used in scientific applications and has a well-maintained homepage at *http://www.qhull.org/*. Another choice is Ken Clarkson's higher-dimensional convex-hull code, *Hull*, available at *http://www.netlib.org/voronoi/hull.html*.

Notes: Voronoi diagrams were studied by Dirichlet in 1850 and are occasionally referred to as *Dirichlet tessellations*. They are named after G. Voronoi, who discussed them in a 1908 paper. In mathematics, concepts get named after the last person to discover them.

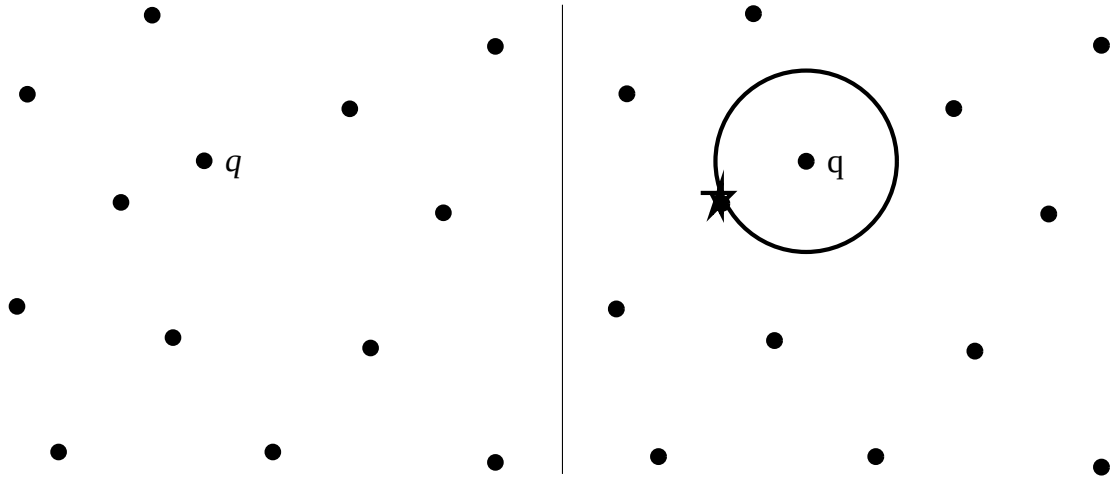
The book by Okabi, et al. [OBSC00] is the most complete treatment of Voronoi diagrams and their applications. Aurenhammer [Aur91] and Fortune [For04] provide excellent surveys on Voronoi diagrams and associated variants such as power diagrams. The first $O(n \lg n)$ algorithm for constructing Voronoi diagrams was based on divide-and-conquer and is due to Shamos and Hoey [SH75]. Good expositions of both Fortune's sweepline algorithm [For87] for constructing Voronoi diagrams in $O(n \lg n)$ and the relationship

between Delaunay triangulations and $(d+1)$-dimensional convex hulls [ES86] include [dBvKOS00, O'R01].

In a kth-order Voronoi diagram, we partition the plane such that each point in a region is closest to the same set of k sites. Using the algorithm of [ES86], the complete set of kth-order Voronoi diagrams can be constructed in $O(n^3)$ time. By doing point location on this structure, the k nearest neighbors to a query point can be found in $O(k + \lg n)$. Expositions on kth-order Voronoi diagrams include [O'R01, PS85].

The smallest enclosing circle problem can be solved in $O(n \lg n)$ time using $(n-1)$st order Voronoi diagrams [PS85]. In fact, there exists a linear-time algorithm based on low-dimensional linear programming [Meg83]. A linear algorithm for computing the Voronoi diagram of a convex polygon is given by [AGSS89].

Related Problems: Nearest neighbor search (see page 580), point location (see page 587), triangulation (see page 572).



INPUT OUTPUT

17.5 Nearest Neighbor Search

Input description: A set S of n points in d dimensions; a query point q.

Problem description: Which point in S is closest to q?

Discussion: The need to quickly find the nearest neighbor of a query point arises in a variety of geometric applications. The classic example involves designing a system to dispatch emergency vehicles to the scene of a fire. Once the dispatcher learns the location of the fire, she uses a map to find the firehouse closest to this point to minimize transportation delays. This situation occurs in any application mapping customers to service providers.

A nearest-neighbor search is also important in classification. Suppose we are given a collection of numerical data about people (say age, height, weight, years of education, and income level) each of whom has been labeled as Democrat or Republican. We seek a classifier to decide which way a given person is likely to vote. Each of the people in our data set is represented by a party-labeled point in d-dimensional space. A simple classifier can be built by assigning the new point to the party affiliation of its nearest neighbor.

Such nearest-neighbor classifiers are widely used, often in high-dimensional spaces. The vector-quantization method of image compression partitions an image into 8×8 pixel regions. This method uses a predetermined library of several thousand 8×8 pixel tiles and replaces each image region by the most similar library tile. The most similar tile is the point in 64-dimensional space that is closest to

the image region in question. Compression is achieved by reporting the identifier of the closest library tile instead of the 64 pixels, at some loss of image fidelity.

Issues arising in nearest-neighbor search include:

- *How many points are you searching?* – When your data set contains only a small number of points (say $n \leq 100$), or if only a few queries are ever destined to be performed, the simple approach is best. Compare the query point q against each of the n data points. Only when fast queries are needed for large numbers of points does it pay to consider more sophisticated methods.

- *How many dimensions are you working in?* – A nearest neighbor search gets progressively harder as the dimensionality increases. The *kd*-tree data structure, presented in Section 12.6 (page 389), does a very good job in moderate-dimensional spaces—even the plane. Still, above 20 dimensions or so, kd-tree search degenerates pretty much to a linear search through the data points. Searches in high-dimensional spaces become hard because a sphere of radius r, representing all the points with distance $\leq r$ from the center, progressively fills up less volume relative to a cube as the dimensionality increases. Thus, any data structure based on partitioning points into enclosing volumes will become progressively less effective.

  In two dimensions, Voronoi diagrams (see Section 17.4 (page 576)) provide an efficient data structure for nearest-neighbor queries. The Voronoi diagram of a point set in the plane decomposes the plane into regions such that the cell containing data point p consists of all points that are nearer to p than any other point in S. Finding the nearest neighbor of query point q reduces to finding which Voronoi diagram cell contains q and reporting the data point associated with it. Although Voronoi diagrams can be built in higher dimensions, their size rapidly grows to the point of unusability.

- *Do you really need the exact nearest neighbor?* – Finding the exact nearest neighbor in a very high dimensional space is hard work; indeed, you probably won't do better than a linear (brute force) search. However, there are algorithms/heuristics that can give you a reasonably close neighbor of your query point fairly quickly.

  One important technique is *dimension reduction*. Projections exist that map any set of n points in d-dimensions into a $d' = O(\lg n/\epsilon^2)$-dimensional space such that distance to the nearest neighbor in the low-dimensional space is within $(1+\epsilon)$ times that of the actual nearest neighbor. Projecting the points onto a random hyperplane of dimension d' in E^d will likely do the trick.

  Another idea is adding some randomness when you search your data structure. A *kd*-tree can be efficiently searched for the cell containing the query point q—a cell whose boundary points are good candidates to be close neighbors. Now suppose we search for a point q', which is a small random perturbations of q. It should land in a different but nearby cell, one of whose

boundary points might prove to be an even closer neighbor of q. Repeating such random queries gives us a way to productively use exactly as much computing time as we are willing to spend to improve the answer.

- *Is your data set static or dynamic?* – Will there be occasional insertions or deletions of new data points in your application? If these are very rare events, it might pay to rebuild your data structure from scratch each time. If they are frequent, select a version of the kd-tree that supports insertions and deletions.

The nearest neighbor graph on a set S of n points links each vertex to its nearest neighbor. This graph is a subgraph of the Delaunay triangulation, and so can be computed in $O(n \log n)$. This is quite a bargain, since it takes $\Theta(n \log n)$ time just to discover the closest pair of points in S.

As a lower bound, the closest-pair problem reduces to sorting in one dimension. In a sorted set of numbers, the closest pair corresponds to two numbers that lie next to each other, so we need only check that which is the minimum gap between the $n - 1$ adjacent pairs. The limiting case occurs when the closest pair are zero distance apart, meaning that the elements are not unique.

Implementations: *ANN* is a C++ library for both exact and approximate nearest neighbor searching in arbitrarily high dimensions. It performs well for searches over hundreds of thousands of points in up to about 20 dimensions. It supports all l_p distance norms, including Euclidean and Manhattan distance, and is available at *http://www.cs.umd.edu/~mount/ANN/*. It is the first code I would turn to for nearest neighbor search.

Samet's spatial index demos (*http://donar.umiacs.umd.edu/quadtree/*) provide a series of Java applets illustrating many variants of *kd*-trees, in association with [Sam06]. *KDTREE 2* contains C++ and Fortran 95 implementations of *kd*-trees for efficient nearest nearest neighbor search in many dimensions. See *http://arxiv.org/abs/physics/0408067*.

Ranger [MS93] is a tool for visualizing and experimenting with nearest-neighbor and orthogonal-range queries in high-dimensional data sets, using multidimensional search trees. Four different search data structures are supported by *Ranger*: naive kd-trees, median kd-trees, nonorthogonal kd-trees, and the vantage point tree. It is available in the algorithm repository *http://www.cs.sunysb.edu/~algorith*.

Nearpt3 is a special-purpose code for nearest-neighbor search of extremely large point sets in three dimensions. See *http://wrfranklin.org/Research/nearpt3*.

See Section 17.4 (page 576) for a complete collection of Voronoi diagram implementations. In particular, CGAL (*www.cgal.org*) and LEDA (see Section 19.1.1 (page 658)) provide implementations of Voronoi diagrams in C++, as well as planar point location to make effective use of them for nearest-neighbor search.

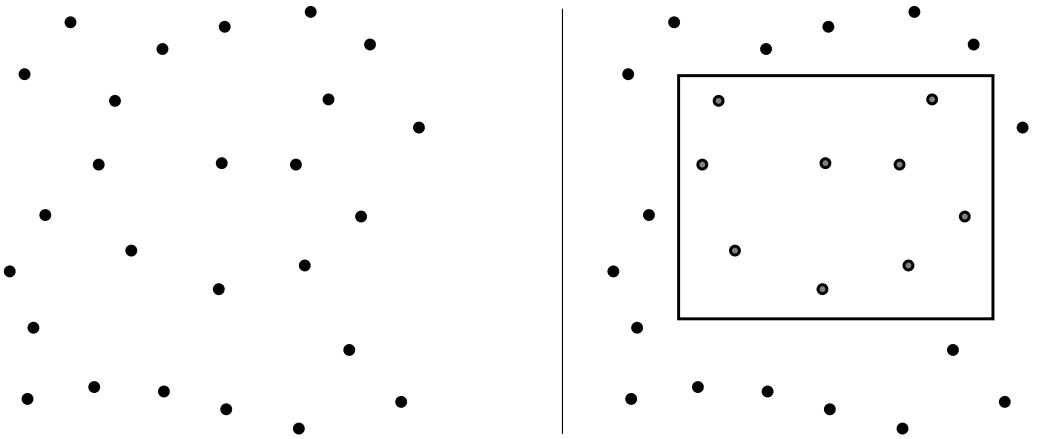
Notes: Indyk [Ind04] ably surveys recent results in approximate nearest neighbor search in high dimensions based on random projection methods. Both theoretical [IM04] and empirical [BM01] results indicate that the method preserves distances quite nicely.

The theoretical guarantees underlying Ayra and Mount's approximate nearest neighbor code *ANN* [AM93, AMN+98] are somewhat different. A sparse weighted graph structure is built from the data set, and the nearest neighbor is found by starting at a random point and greedily walking towards the query point in the graph. The closest point found over several random trials is declared the winner. Similar data structures hold promise for other problems in high-dimensional spaces. Nearest-neighbor search was a subject of the Fifth DIMACS challenge, as reported in [GJM02].

Samet [Sam06] is the best reference on kd-trees and other spatial data structures. All major (and many minor) variants are developed in substantial detail. A shorter survey [Sam05] is also available. The technique of using random perturbations of the query point is due to [Pan06].

Good expositions on finding the closest pair of points in the plane [BS76] include [CLRS01, Man89]. These algorithms use a divide-and-conquer approach instead of just selecting from the Delaunay triangulation.

Related Problems: Kd-trees (see page 389), Voronoi diagrams (see page 576), range search (see page 584).



INPUT OUTPUT

17.6 Range Search

Input description: A set S of n points in E^d and a query region Q.

Problem description: What points in S lie within Q?

Discussion: Range-search problems arise in database and geographic information system (GIS) applications. Any data object with d numerical fields, such as person with height, weight, and income, can be modeled as a point in d-dimensional space. A *range query* describes a region in space and asks for all points or the number of points in the region. For example, asking for all people with income between \$0 and \$10,000, with height between 6'0" and 7'0", and weight between 50 and 140 lbs., defines a box containing people whose wallet and body are both thin.

The difficulty of range search depends on several factors:

- *How many range queries are you going to perform?* – The simplest approach to range search tests each of the n points one by one against the query polygon Q. This works just fine when the number of queries will be small. Algorithms to test whether a point is within a given polygon are presented in Section 17.7 (page 587).

- *What shape is your query polygon?* – The easiest regions to query against are *axis-parallel rectangles*, because the inside/outside test reduces to verifying whether each coordinate lies within a prescribed range. The input-output figure illustrates such an *orthogonal range query.*

When querying against a nonconvex polygon, it will pay to partition your polygon into convex pieces or (even better) triangles and then query the point set against each one of the pieces. This works because it is quick and easy to test whether a point lies inside a convex polygon. Algorithms for such convex decompositions are discussed in Section 17.11 (page 601).

- *How many dimensions?* – A general approach to range queries builds a kd-tree on the point set, as discussed in Section 12.6 (page 389). A depth-first traversal of the kd-tree is performed for the query, with each tree node expanded only if the associated rectangle intersects the query region. The entire tree might have to be traversed for sufficiently large or misaligned query regions, but in general kd-trees lead to an efficient solution. Algorithms with more efficient worst-case performance are known in two dimensions, but kd-trees are likely to work just fine in the plane. In higher dimensions, they provide the only viable solution to the problem.

- *Is your point set static, or might there be insertions/deletions?* – A clever practical approach to range search and many other geometric searching problems is based on Delaunay triangulations. Delaunay triangulation edges connect each point p to nearby points, including its nearest neighbor. To perform a range query, we start by using planar point location (see Section 17.7 (page 587)) to quickly identify a triangle within the region of interest. We then do a depth-first search around a vertex of this triangle, pruning the search whenever it visits a point too distant to have interesting undiscovered neighbors. This should be efficient, because the total number of points visited should be roughly proportional to the number within the query region.

  One nice thing about this approach is that it is relatively easy to employ "edge-flip" operations to fix up a Delaunay triangulation following a point insertion or deletion. See Section 17.3 (page 572) for more details.

- *Can I just count the number of points in a region, or do I have to identify them?* – For many applications, it suffices to count the number of points in a region instead of returning them. Harkening back to the introductory example, we may want to know whether there are more thin/poor people or rich/fat ones. The need to find the densest or emptiest region in space often arises, and this problem can be solved by counting range queries.

  A nice data structure for efficiently answering such aggregate range queries is based on the dominance ordering of the point set. A point x is said to *dominate* point y if y lies both below and to the left of x. Let $DOM(p)$ be a function that counts the number of points in S that are dominated by p. The number of points m in the orthogonal rectangle defined by $x_{\min} \leq x \leq x_{\max}$ and $y_{\min} \leq y \leq y_{\max}$ is given by

$$m = DOM(x_{\max}, y_{\max}) - DOM(x_{\max}, y_{\min}) - DOM(x_{\min}, y_{\max}) + DOM(x_{\min}, y_{\min})$$

The second additive term corrects for the points for the lower left-hand corner that have been subtracted away twice.

To answer arbitrary dominance queries efficiently, partition the space into n^2 rectangles by drawing a horizontal and vertical line through each of the n points. The set of dominated points is identical for each point in any rectangle, so the dominance count of the lower left-hand corner of each rectangle can be precomputed, stored, and reported for any query point within it. Range queries reduce to binary search and thus take $O(\lg n)$ time. Unfortunately, this data structure takes quadratic space. However, the same idea can be adapted to kd-trees to create a more space-efficient search structure.

Implementations: Both CGAL (*www.cgal.org*) and LEDA (see Section 19.1.1 (page 658)) use a dynamic Delaunay triangulation data structure to support circular, triangular, and orthogonal range queries. Both libraries also provide implementations of range tree data structures, which support orthogonal range queries in $O(k + \lg^2 n)$ time where n is the complexity of the subdivision and k is the number of points in the rectangular region.

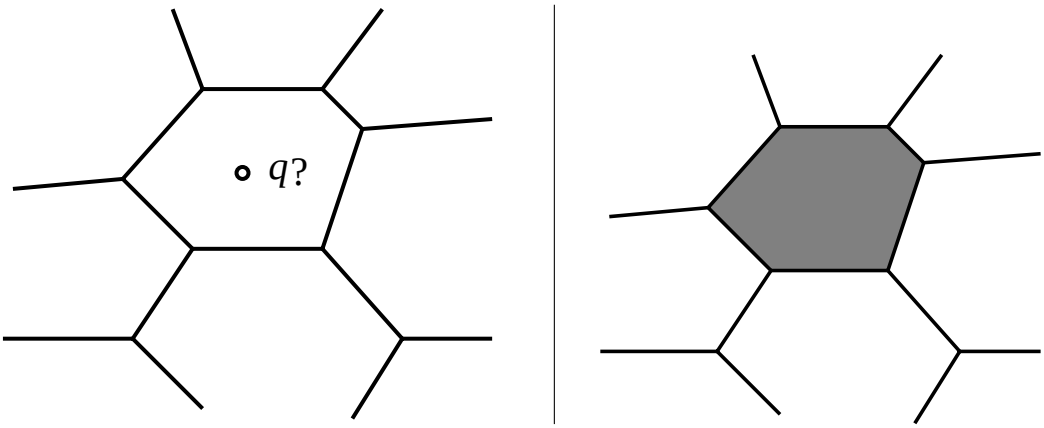
ANN is a C++ library for both exact and approximate nearest neighbor searching in arbitrarily high dimensions. It performs well for searches over hundreds of thousands of points in up to about 20 dimensions. It supports fixed-radius, nearest-neighbor queries over all l_p distance norms, which can be used to approximate circular and orthogonal range queries under the l_2 and l_1 norms, respectively. *ANN* is available at *http://www.cs.umd.edu/∼mount/ANN/*.

Ranger is a tool for visualizing and experimenting with nearest-neighbor and orthogonal-range queries in high-dimensional data sets, using multidimensional search trees. Four different search data structures are supported by *Ranger*: naive kd-trees, median kd-trees, nonorthogonal kd-trees, and the vantage point tree. For each of these, *Ranger* supports queries in up to 25 dimensions under any Minkowski metric. It is available in the algorithm repository.

Notes: Good expositions on data structures with worst-case $O(\lg n + k)$ performance for orthogonal-range searching [Wil85] include [dBvKOS00, PS85]. Exposition on *kd*-trees for orthogonal range queries in two dimensions appear in [dBvKOS00, PS85]. Their worst-case performance can be very bad; [LW77] describes an instance in two dimensions requiring $O(\sqrt{n})$ time to report that a rectangle is empty.

The problem becomes considerably more difficult for nonorthogonal range queries, where the query region is not an axis-aligned rectangle. For half-plane intersection queries, $O(\lg n)$ time and linear space suffice [CGL85]; for range searching with simplex query regions (such as a triangle in the plane), lower bounds preclude efficient worst-case data structures. See Agrawal [Aga04] for a survey and discussion.

Related Problems: Kd-trees (see page 389), point location (see page 587).



INPUT OUTPUT

17.7 Point Location

Input description: A decomposition of the plane into polygonal regions and a query point q.

Problem description: Which region contains the query point q?

Discussion: Point location is a fundamental subproblem in computational geometry, usually needed as an ingredient to solve larger geometric problems. In a typical police dispatch system, the city will be partitioned into different precincts or districts. Given a map of regions and a query point (the crime scene), the system must identify which region contains the point. This is exactly the problem of planar point location. Variations include:

- *Is a given point inside or outside of polygon P?* – The simplest version of point location involves only two regions, inside-P and outside-P, and asks which contains a given query point. For polygons with lots of narrow spirals, this can be surprisingly difficult to tell by inspection. The secret to doing it both by eye or machine is to draw a ray starting from the query point and ending beyond the furthest extent of the polygon. Count the number of times the polygon crosses through an edge. The query point will lie within the polygon iff this number is odd. The case of the line passing through a vertex instead of an edge is evident from context, since we are counting the number of times we pass through the boundary of the polygon. Testing each of the n edges for intersection against the query ray takes $O(n)$ time. Faster

algorithms for convex polygons are based on binary search, and take $O(\lg n)$ time.

- *How many queries must be performed?* – It is always possible to perform this inside-polygon test separately on each region in a given planar subdivision. However, it would be wasteful to perform many such point location queries on the same subdivision. It would be much better to construct a grid-like or tree-like data structure on top of our subdivision to get us near the correct region quickly. Such search structures are discussed in more detail below.

- *How complicated are the regions of your subdivision?* – More sophisticated inside-outside tests are required when the regions of your subdivision are arbitrary polygons. By triangulating all polygonal regions first, each inside-outside test reduces to testing whether a point is in a triangle. Such tests can be made particularly fast and simple, at the minor cost of recording the full polygon name for each triangle. An added benefit is that the smaller your regions are, the better grid-like or tree-like superstructures are likely to perform. Some care should be taken when you triangulate to avoid long skinny triangles, as discussed in Section 17.3 (page 572).

- *How regularly sized and spaced are your regions?* – If all resulting triangles are about the same size and shape, the simplest point location method imposes a regularly-spaced $k \times k$ grid of horizontal and vertical lines over the entire subdivision. For each of the k^2 rectangular regions, we maintain a list of all the regions that are at least partially contained within the rectangle. Performing a point location query in such a *grid file* involves a binary search or hash table lookup to identify which rectangle contains query point q, and then searching each region in the resulting list to identify the right one.

  Such grid files can perform very well, provided that each triangular region overlaps only a few rectangles (thus minimizing storage space) and each rectangle overlaps only a few triangles (thus minimizing search time). Whether it performs well depends on the regularity of your subdivision. Some flexibility can be achieved by spacing the horizontal lines irregularly, depending upon where the regions actually lie. The *slab method*, discussed below, is a variation on this idea that guarantees worst-case efficient point location at the cost of quadratic space.

- *How many dimensions will you be working in?* – In three or more dimensions, some flavor of kd-tree will almost certainly be the point-location method of choice. They may also be the right answer for planar subdivisions that are too irregular for grid files.

  Kd-trees, described in Section 12.6 (page 389), decompose the space into a hierarchy of rectangular boxes. At each node in the tree, the current box is split into a small number (typically 2, 4, or 2^d for dimension d) of smaller boxes. Each leaf box is labeled with the (small) set regions that are at least

partially contained in the box. The point location search starts at the root of the tree and keeps traversing down the child whose box contains the query point q. When the search hits a leaf, we test each of the relevant regions to see which one of them contains q. As with grid files, we hope that each leaf contains a small number of regions and that each region does not cut across too many leaf cells.

- *Am I close to the right cell?* – Walking is a simple point-location technique that might even work well beyond two dimensions. Start from an arbitrary point p in an arbitrary cell, hopefully close to the query point q. Construct the line (or ray) from p to q and identify which face of the cell this hits (a so-called *ray shooting query*). Such queries take constant time in triangulated arrangements.

  Proceeding to the neighboring cell through this face gets us one step closer to the target. The expected path length will be $O(n^{1/d})$ for sufficiently regular d-dimensional arrangements, although linear in the worst case.

The simplest algorithm to guarantee $O(\lg n)$ worst-case access is the *slab* method, which draws horizontal lines through each vertex, thus creating $n + 1$ "slabs" between the lines. Since the slabs are defined by horizontal lines, finding the slab containing a particular query point can be done using a binary search on the y-coordinate of q. Since there can be no vertices within any slab, the region containing a point within a slab can be identified by a second binary search on the edges that cross the slab. The catch is that a binary search tree must be maintained for each slab, for a worst-case of $O(n^2)$ space. A more space-efficient approach based on building a hierarchy of triangulations over the regions also achieves $O(\lg n)$ for search and is discussed in the notes below.

Worst-case efficient computational geometry methods either require a lot of storage or are fairly complicated to implement. We identify implementations of worst-case methods below, which are worth at least experimenting with. However, we recommend kd-trees for most general point-location applications.

Implementations: Both CGAL (*www.cgal.org*) and LEDA (see Section 19.1.1 (page 658)) provide excellent support for maintaining planar subdivisions in C++. CGAL favors a jump-and-walk strategy, although a worst-case logarithmic search is also provided. LEDA implements expected $O(\lg n)$ point location using partially persistent search trees.

ANN is a C++ library for both exact and approximate nearest-neighbor searching in arbitrarily high dimensions. It can be used to quickly identify a nearby cell boundary point to begin walking from. Check it out at *http://www.cs.umd.edu/~mount/ANN/*.

Arrange is a package for maintaining arrangements of polygons in either the plane or on the sphere. Polygons may be degenerate, and hence represent arrangements of lines. A randomized incremental construction algorithm is used, and efficient point location on the arrangement is supported.

Arrange is written in C by Michael Goldwasser and is available from *http://euler.slu.edu/∼goldwasser/publications/*.

Routines (in C) to test whether a point lies in a simple polygon have been provided by [O'R01, SR03].

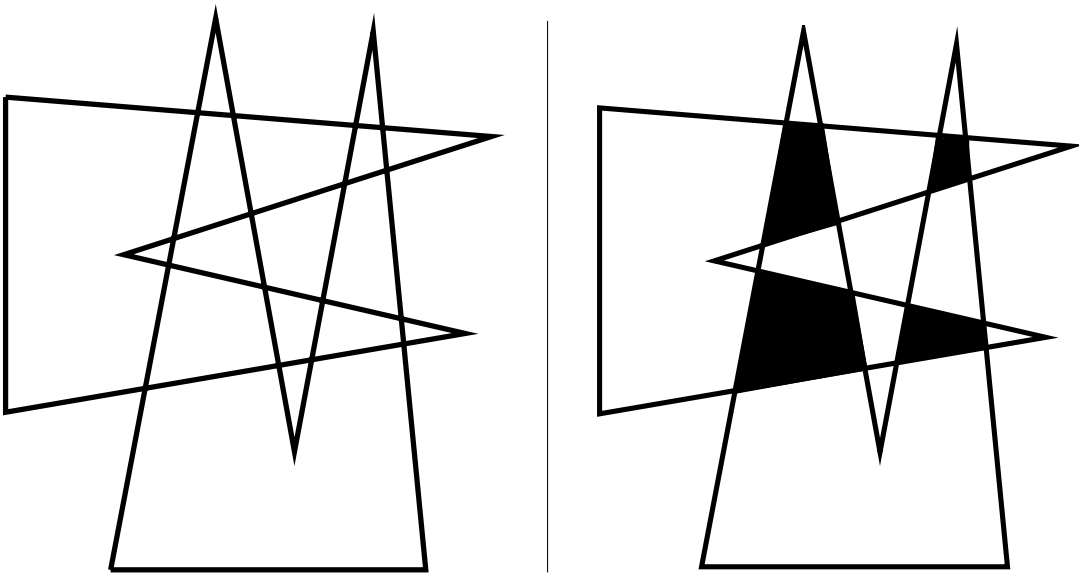
Notes: Snoeyink [Sno04] gives an excellent survey of the state-of-the-art in point location, both theoretical and practical. Very thorough treatments of deterministic planar-point location data structures are provided by [dBvKOS00, PS85].

Tamassia and Vismara [TV01] use planar point location as a case study of geometric algorithm engineering, in Java. An experimental study of algorithms for planar point location is described in [EKA84]. The winner was a bucketing technique akin to the grid file.

The elegant triangle refinement method of Kirkpatrick [Kir83] builds a hierarchy of triangulations above the actual planar subdivision such that each triangle on a given level intersects only a constant number of triangles on the following level. Since each triangulation is a fraction of the size of the subsequent one, the total space is obtained by summing up a geometric series and hence is linear. Furthermore, the height of the hierarchy is $O(\lg n)$, ensuring fast query times. An alternative algorithm realizing the same time bounds is [EGS86]. The slab method described above is due to [DL76] and is presented in [PS85]. Expositions on the inside-outside test for simple polygons include [Hai94, O'R01, PS85, SR03].

More recently, there has been interest in dynamic data structures for point location, which support fast incremental updates of the planar subdivision (such as insertions and deletions of edges and vertices) as well as fast point location. Chiang and Tamassia's [CT92] survey is an appropriate place to begin, with updated references in [Sno04].

Related Problems: Kd-trees (see page 389), Voronoi diagrams (see page 576), nearest neighbor search (see page 580).



INPUT OUTPUT

17.8 Intersection Detection

Input description: A set S of lines and line segments $l_1, \ldots, l_n$ or a pair of polygons or polyhedra P_1 and P_2.

Problem description: Which pairs of line segments intersect each other? What is the intersection of P_1 and P_2?

Discussion: Intersection detection is a fundamental geometric primitive with many applications. Picture a virtual-reality simulation of an architectural model for a building. The illusion of reality vanishes the instant the virtual person walks through a virtual wall. To enforce such physical constraints, any such intersection between polyhedral models must be immediately detected and the operator notified or constrained.

Another application of intersection detection is design rule checking for VLSI layouts. A minor design defect resulting in two crossing metal strips could short out the chip, but such errors can be detected before fabrication, using programs to find all intersections between line segments.

Issues arising in intersection detection include:

- *Do you want to compute the intersection or just report it?* – We distinguish between intersection detection and computing the actual intersection.

Detecting that an intersection exists can be substantially easier, and often suffices. For the virtual-reality application, it might not be important to know exactly where we hit the wall—just that we hit it.

- *Are you intersecting lines or line segments?* – The big difference here is that any two lines with different slopes intersect in at exactly one point. All the points of intersections can be found in $O(n^2)$ time by comparing each pair of lines. Constructing the arrangement of the lines provides more information than just the intersection points, and is discussed in Section 17.15 (page 614).

  Finding all the intersections between n line segments is considerably more challenging. Even the basic primitive of testing whether two line segments intersect is not as trivial, as discussed in Section 17.1 (page 564). Of course, we could explicitly test each line segment pair and thus find all intersections in $O(n^2)$ time, but faster algorithms exist when there are few intersection points.

- *How many intersection points do you expect?* – In VLSI design-rule checking, we expect the set of line segments to have few if any intersections. What we seek is an algorithm whose time is *output sensitive*, taking time proportional to the number of intersection points.

  Such output-sensitive algorithms exist for line-segment intersection. The fastest algorithm takes $O(n \lg n + k)$ time, where k is the number of intersections. These algorithms are based on the planar sweepline approach.

- *Can you see point x from point y?* – Visibility queries ask whether vertex x can see vertex y unobstructed in a room full of obstacles. This can be phrased as the following line-segment intersection problem: does the line segment from x to y intersect any obstacle? Such visibility problems arise in robot motion planning (see Section 17.14) and in hidden-surface elimination for computer graphics.

- *Are the intersecting objects convex?* – Better intersection algorithms exist when the line segments form the boundaries of polygons. The critical issue here becomes whether the polygons are convex. Intersecting a convex n-gon with a convex m-gon can be done in $O(n + m)$ time, using the sweepline algorithm discussed next. This is possible because the intersection of two convex polygons must form another convex polygon with at most $n + m$ vertices.

  However, the intersection of two nonconvex polygons is not so well behaved. Consider the intersection of two "combs" generalizing the Picasso-like frontspiece to this section. As illustrated, the intersection of nonconvex polygons may be disconnected and have quadratic size in the worst case.

Intersecting polyhedra is more complicated than polygons, because two polyhedra can intersect even when no edges do. Consider the example of a needle piercing the interior of a face. In general, however, the same issues arise for both polygons and polyhedra.

- *Are you searching for intersections repeatedly with the same basic objects?* – In the walk-through application just described, the room and the objects in it don't change between one scene and the next. Only the person moves, and intersections are rare.

  One common technique is to approximate the objects in the scene by simpler objects that enclose them, such as boxes. Whenever two enclosing boxes intersect, then the underlying objects *might* intersect, and so further work is necessary to decide the issue. However, it is much more efficient to test whether simple boxes intersect than more complicated objects, so we win if collisions are rare. Many variations on this theme are possible, but this idea leads to large performance improvements for complicated environments.

Planar sweep algorithms can be used to efficiently compute the intersections among a set of line segments, or the intersection/union of two polygons. These algorithms keep track of interesting changes as we sweep a vertical line from left to right over the data. At its leftmost position, the line intersects nothing, but as it moves to the right, it encounters a series of events:

- *Insertion* – The leftmost point of a line segment may be encountered, and it is now available to intersect some other line segment.

- *Deletion* – The rightmost point of a line segment is encountered. This means that we have completely swept over the segment, and so it can be deleted from further consideration.

- *Intersection* – If the active line segments that intersect the sweep line are maintained as sorted from top to bottom, the next intersection must occur between neighboring line segments. After this intersection, these two line segments swap their relative order.

Keeping track of what is going on requires two data structures. The future is maintained by an *event queue*, or a priority queue ordered by the x-coordinate of all possible future events of interest: insertion, deletion, and intersection. See Section 12.2 (page 373) for priority queue implementations. The present is represented by the *horizon*—an ordered list of line segments intersecting the current position of the sweepline. The horizon can be maintained using any dictionary data structure, such as a balanced tree.

To adapt this approach to compute the intersection or union of polygons, we modify the processing of the three basic event types. This algorithm can be considerably simplified for pairs of convex polygons, since (1) at most four polygon

edges intersect the sweepline, so no horizon data structure is needed, and (2) no event-queue sorting is needed, since we can start from the leftmost vertex of each polygon and proceed to the right by following the polygonal ordering.

Implementations: Both LEDA (see Section 19.1.1 (page 658)) and CGAL (*www.cgal.org*) offers extensive support for line segment and polygonal intersection. In particular, they provide a C++ implementation of the Bentley-Ottmann sweepline algorithm [BO79], finding all k intersection points between n line segments in the plane in $O((n+k)\lg n)$ time.

O'Rourke [O'R01] provides a robust program in C to compute the intersection of two convex polygons. See Section 19.1.10 (page 662).

The University of North Carolina GAMMA group has produced several efficient collision detection libraries, of which *SWIFT++* [EL01] is the most recent member. It can detect intersection, compute approximate/exact distances between objects, and determine object-pair contacts in scenes composed of rigid polyhedral models. See *http://www.cs.unc.edu/∼geom/collide/* for pointers to all of these libraries.

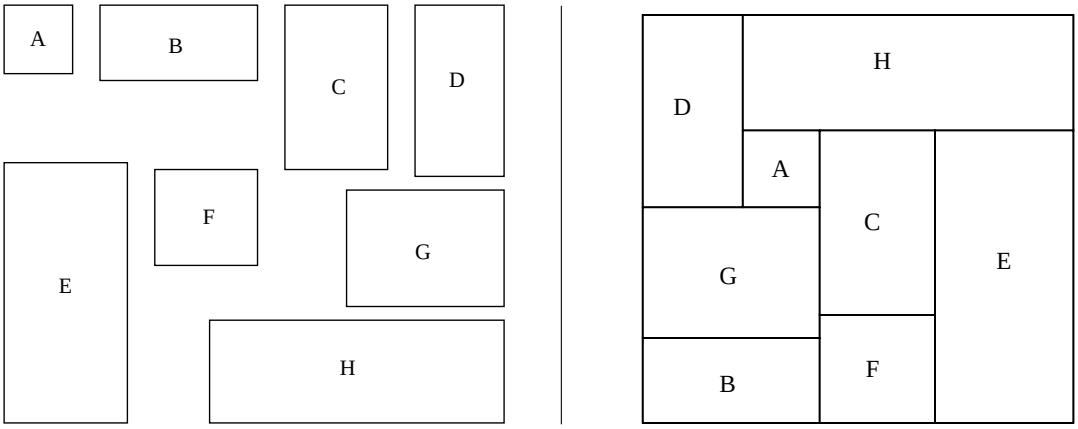
Finding the mutual intersection of a collection of half-spaces is a special case of the convex-hulls, and Qhull [BDH97] is convex hull code of choice for general dimensions. Qhull has been widely used in scientific applications and has a well-maintained homepage at *http://www.qhull.org/*.

Notes: Mount [Mou04] is an excellent survey of algorithms for computing intersections of geometric objects such as line segments, polygons, and polyhedra. Books with chapters discussing such problems include [dBvKOS00, CLRS01, PS85]. Preparata and Shamos [PS85] provide a good exposition on the special case of finding intersections and unions of axis-oriented rectangles—a problem that arises often in VLSI design.

An optimal $O(n \lg n + k)$ algorithm for computing line segment intersections is due to Chazelle and Edelsbrunner [CE92]. Simpler, randomized algorithms achieving the same time bound are thoroughly presented by Mulmuley [Mul94].

Lin and Manocha [LM04] survey techniques and software for collision detection.

Related Problems: Maintaining arrangements (see page 614), motion planning (see page 610).



17.9 Bin Packing

Input description: A set of n items with sizes $d_1, \ldots, d_n$. A set of m bins with capacity $c_1, \ldots, c_m$.

Problem description: Store all the items using the smallest number of bins.

Discussion: Bin packing arises in a variety of packaging and manufacturing problems. Suppose that you are manufacturing widgets cut from sheet metal or pants cut from cloth. To minimize cost and waste, we seek to lay out the parts so as to use as few fixed-size metal sheets or bolts of cloth as possible. Identifying which part goes on which sheet in which location is a bin-packing variant called the *cutting stock* problem. Once our widgets have been successfully manufactured, we are faced with another bin-packing problem—namely how best to fit the boxes into trucks to minimize the number of trucks needed to ship everything.

Even the most elementary-sounding bin-packing problems are NP-complete; see the discussion of integer partition in Section 13.10 (page 427). Thus, we are doomed to think in terms of heuristics instead of worst-case optimal algorithms. Fortunately, relatively simple heuristics tend to work well on most bin-packing problems. Further, many applications have peculiar, problem-specific constraints that tend to frustrate sophisticated algorithms for bin packing. The following factors will affect the choice of heuristic:

- *What are the shapes and sizes of the objects?* – The character of a bin-packing problem depends greatly on the shapes of the objects to be packed. Solving a standard jigsaw puzzle is a much different problem than packing squares

into a rectangular box. In *one-dimensional bin packing*, each object's size is given simply as an integer. This is equivalent to packing boxes of equal width into a chimney of that width, and makes it a special case of the knapsack problem of Section 13.10 (page 427).

When all the boxes are of identical size and shape, repeatedly filling each row gives a reasonable, but not necessarily optimal, packing. Consider trying to fill a 3×3 square with 2×1 bricks. You can only pack three bricks using one orientation, while four bricks suffice with two.

- *Are there constraints on the orientation and placement of objects?* – Many boxes are labeled "this side up" (imposing an orientation on the box) or "do not stack" (requiring them sit on top of any box pile). Respecting these constraints restricts our flexibility in packing and hence will increase in the number of trucks needed to send out certain shipments. Most shippers solve the problem by ignoring the labels. Indeed, your task will be simpler if you don't have to worry about the consequences of them.

- *Is the problem on-line or off-line?* – Do we know the complete set of objects to pack at the beginning of the job (an *off-line* problem)? Or will we get them one at a time and deal with them as they arrive (an *on-line* problem)? The difference is important, because we can do a better job packing when we can take a global view and plan ahead. For example, we can arrange the objects in an order that will facilitate efficient packing, perhaps by sorting them from biggest to smallest.

The standard off-line heuristics for bin packing order the objects by size or shape and then insert them into bins. Typical insertion rules are (1) select the first or leftmost bin the object fits in, (2) select the bin with the most room, (3) select the bin that provides the tightest fit, or (4) select a random bin.

Analytical and empirical results suggest that *first-fit decreasing* is the best heuristic. Sort the objects in decreasing order of size, so that the biggest object is first and the smallest last. Insert each object one by one into the first bin that has room for it. If no bin has room, we must start another bin. In the case of one-dimensional bin packing, this can never require more than 22% more bins than necessary and usually does much better. First-fit decreasing has an intuitive appeal to it, for we pack the bulky objects first and hope that little objects can fill up the cracks.

First-fit decreasing is easily implemented in $O(n \lg n + bn)$ time, where $b \leq \min(n, m)$ is the number of bins actually used. Simply do a linear sweep through the bins on each insertion. A faster $O(n \lg n)$ implementation is possible by using a binary tree to keep track of the space remaining in each bin.

We can fiddle with the insertion order in such a scheme to deal with problem-specific constraints. For example, it is reasonable to take "do not stack" boxes last (perhaps after artificially lowering the height of the bins to leave some room up

top to work with) and to place fixed-orientation boxes at the beginning (so we can use the extra flexibility later to stick boxes on top).

Packing boxes is much easier than packing arbitrary geometric shapes, enough so that a general approach packs each part into its own box and then packs the boxes. Finding an enclosing rectangle for a polygonal part is easy; just find the upper, lower, left, and right tangents in a given orientation. Finding the orientation and minimizing the area (or volume) of such a box is more difficult, but can be done in both two and three dimensions [O'R85]. See the Implementations section for a fast approximation to minimum enclosing box.

In the case of nonconvex parts, considerable useful space can be wasted in the holes created by placing the part in a box. One solution is to find the *maximum empty rectangle* within each boxed part and use this to contain other parts if it is sufficiently large. More advanced solutions are discussed in the references.

Implementations: Martello and Toth's collection of Fortran implementations of algorithms for a variety of knapsack problem variants are available at *http://www.or.deis.unibo.it/kp.html*. An electronic copy of [MT90a] has also been generously made available.

David Pisinger maintains a well-organized collection of C-language codes for knapsack problems and related variants like bin packing and container loading. These are available at *http://www.diku.dk/∼pisinger/codes.html*.

A first step towards packing arbitrary shapes packs each in its own minimum volume box. For a code to find an approximation to the optimal packing, see *http://valis.cs.uiuc.edu/∼sariel/research/papers/00/diameter/diam_prog.html*. This algorithm runs in near-linear time [BH01].

Notes: See [CFC94, CGJ96, LMM02] for surveys of the extensive literature on bin packing and the cutting stock problem. Keller, Pferschy, and Psinger [KPP04] is the most current reference on the knapsack problem and variants. Experimental results on bin-packing heuristics include [BJLM83, MT87].

Efficient algorithms are known for finding the largest empty rectangle in a polygon [DMR97] and point set [CDL86].

Sphere packing is an important and well-studied special case of bin packing, with applications to error-correcting codes. Particularly notorious was the "Kepler conjecture"—the problem of establishing the densest packing of unit spheres in three dimensions. This conjecture was finally settled by Hales and Ferguson in 1998; see [Szp03] for an exposition. Conway and Sloane [CS93] is the best reference on sphere packing and related problems.

Milenkovic has worked extensively on two-dimensional bin-packing problems for the apparel industry, minimizing the amount of material needed to manufacture pants and other clothing. Reports of this work include [DM97, Mil97].

Related Problems: Knapsack problem (see page 427), set packing (see page 625).

INPUT OUTPUT

17.10 Medial-Axis Transform

Input description: A polygon or polyhedron P.

Problem description: What are the set of points within P that have more than one closest point on the boundary of P?

Discussion: The medial-axis transformation is useful in *thinning* a polygon, or as is sometimes said, finding its *skeleton*. The goal is to extract a simple, robust representation of the shape of the polygon. The thinned versions of the letters A and B capture the essence of their shape, and would be relatively unaffected by changing the thickness of strokes or by adding font-dependent flourishes such as serifs. The skeleton also represents the center of the given shape, a property that leads to other applications like shape reconstruction and motion planning.

The medial-axis transformation of a polygon is always a tree, making it fairly easy to use dynamic programming to measure the "edit distance" between the skeleton of a known model and the skeleton of an unknown object. Whenever the two skeletons are close enough, we can classify the unknown object as an instance of our model. This technique has proven useful in computer vision and in optical character recognition. The skeleton of a polygon with holes (like the A and B) is not a tree but an embedded planar graph, but it remains easy to work with.

There are two distinct approaches to computing medial-axis transforms, depending upon whether your input is arbitrary geometric points or pixel images:

- *Geometric data* – Recall that the Voronoi diagram of a point set S (see Section 17.4 (page 576)) decomposes the plane into regions around each point $s_i \in S$ such that points within the region around s_i are closer to s_i than to any other site in S. Similarly, the Voronoi diagram of a set of line segments L decomposes the plane into regions around each line segment $l_i \in L$ such that all points within the region around l_i are closer to l_i than to any other site in L.

Any polygon is defined by a collection of line segments such that l_i shares a vertex with l_{i+1}. The medial-axis transform of a polygon P is simply the portion of the line-segment Voronoi diagram that lies within P. Any line-segment Voronoi diagram code thus suffices to do polygon thinning.

The *straight skeleton* is a structure related to the medial axis of a polygon, except that the bisectors are not equidistant to its defining edges but instead to the supporting lines of such edges. The straight skeleton, medial axis and Voronoi diagram are all identical for convex polygons, but in general skeleton bisectors may not be located in the center of the polygon. However, the straight skeleton is quite similar to a proper medial axis transform but is easier to compute. In particular, all edges in a straight skeleton are polygonal. See the Notes section for references with more details on how to compute it.

- *Image data* – Digitized images can be interpreted as points sitting at the lattice points on an integer grid. Thus, we could extract a polygonal description from boundaries in an image and feed it to the geometric algorithms just described. However, the internal vertices of the skeleton will most likely not lie at grid points. Geometric approaches to image processing problems often flounder because images are pixel-based and not continuous.

  A direct pixel-based approach for constructing a skeleton implements the "brush fire" view of thinning. Imagine a fire burning along all edges of the polygon, racing inward at a constant speed. The skeleton is marked by all points where two or more fires meet. The resulting algorithm traverses all the boundary pixels of the object, identifies those vertices as being in the skeleton, deletes the rest of the boundary, and repeats. The algorithm terminates when all pixels are extreme, leaving an object only one or two pixels thick. When implemented properly, this takes linear time in the number of pixels in the image.

  Algorithms that explicitly manipulate pixels tend to be easy to implement, because they avoid complicated data structures. However, the geometry doesn't work out exactly right in such pixel-based approaches. For example, the skeleton of a polygon is no longer always a tree or even necessarily connected, and the points in the skeleton will be close-to-but-not-quite equidistant to two boundary edges. Since you are trying to do continuous geometry in a discrete world, there is no way to solve the problem completely. You just have to live with it.

Implementations: CGAL (*www.cgal.org*) includes a package for computing the straight skeleton of a polygon P. Associated with it are routines for constructing offset contours defining the polygonal regions within P whose points are at least distance d from the boundary.

VRONI [Hel01] is a robust and efficient program for computing Voronoi diagrams of line segments, points, and arcs in the plane. It can readily compute

medial-axis transforms of polygons since it can construct Voronoi diagrams of arbitrary line segments. *VRONI* has been tested on thousands of synthetic and real-world data sets, some with over a million vertices. For more information, see *http://www.cosy.sbg.ac.at/∼held/projects/vroni/vroni.html*. Other programs for constructing Voronoi diagrams are discussed in Section 17.4 (page 576).

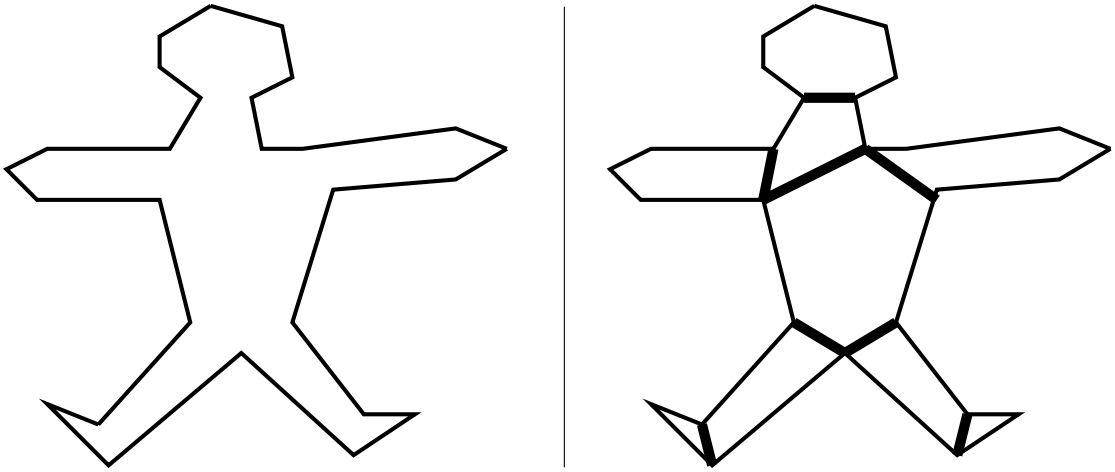
Programs that reconstruct or interpolate point clouds often are based on medial axis transforms. *Cocone* (*http://www.cse.ohio-state.edu/∼tamaldey/cocone.html*) constructs an approximate medial-axis transform of the polyhedral surface it interpolates from points in E^3. See [Dey06] for the theory behind *Cocone*. *Powercrust* [ACK01a, ACK01b] constructs a discrete approximation to the medial-axis transform, and then reconstructs the surface from this transform. When the point samples are sufficiently dense, the algorithm is guaranteed to produce a geometrically and topologically correct approximation to the surface. It is available at *http://www.cs.utexas.edu/users/amenta/powercrust/*.

Notes: For a comprehensive survey of thinning approaches in image processing, see [LLS92, Ogn93]. The medial axis transformation was introduced for shape similarity studies in biology [Blu67]. Applications of the medial-axis transformation in pattern recognition are discussed in [DHS00]. The medial axis transformation is fundamental to the power crust algorithm for surface reconstruction from sampled points; see [ACK01a, ACK01b]. Good expositions on the medial-axis transform include [dBvKOS00, O'R01, Pav82].

The medial-axis of a polygon can be computed in $O(n \lg n)$ time for arbitrary n-gons [Lee82], although linear-time algorithms exist for convex polygons [AGSS89]. An $O(n \lg n)$ algorithm for constructing medial-axis transforms in curved regions was given by Kirkpatrick [Kir79].

Straight skeletons were introduced in [AAAG95], with a subquadratic algorithm due to [EE99]. See [LD03] for an interesting application of straight skeletons to defining the roof structures in virtual building models.

Related Problems: Voronoi diagrams (see page 576), Minkowski sum (see page 617).



INPUT OUTPUT

17.11 Polygon Partitioning

Input description: A polygon or polyhedron P.

Problem description: Partition P into a small number of simple (typically convex) pieces.

Discussion: Polygon partitioning is an important preprocessing step for many geometric algorithms, because geometric problems tend to be simpler on convex objects than on nonconvex ones. It is often easier to work with a small number of convex pieces than with a single nonconvex polygon.

Several flavors of polygon partitioning arise, depending upon the particular application:

- *Should all the pieces be triangles?* – Triangulation is the mother of all polygon partitioning problems, where we partition the interior of the polygon completely into triangles. Triangles are convex and have only three sides, making them the most elementary possible polygon.

  All triangulations of an n-vertex polygon contain exactly $n - 2$ triangles. Therefore, triangulation cannot be the answer if we seek a small number of convex pieces. A "nice" triangulation is judged by the shape of the triangles, not the count. See Section 17.3 (page 572) for a thorough discussion of triangulation.

- *Do I want to cover or partition my polygon?* – *Partitioning* a polygon means completely dividing the interior into nonoverlapping pieces. *Covering* a polygon means that our decomposition is permitted to contain mutually overlapping pieces. Both can be useful in different situations. In decomposing a complicated query polygon in preparation for a range search (Section 17.6 (page 584)), we seek a partitioning, so that each point we locate occurs in exactly one piece. In decomposing a polygon for painting purposes, a covering suffices, since there is no difficulty with filling in a region twice. We will concentrate here on partitioning, since it is simpler to do right, and any application needing a covering will accept a partitioning. The only drawback is that partitions can be larger than coverings.

- *Am I allowed to add extra vertices?* – A final issue is whether we are allowed to add Steiner vertices to the polygon, either by splitting edges or adding interior points. Otherwise, we are restricted to adding chords between two existing vertices. The former may result in a smaller number of pieces, at the cost of more complicated algorithms and perhaps messier results.

The Hertel-Mehlhorn heuristic for convex decomposition using diagonals is simple and efficient. It starts with an arbitrary triangulation of the polygon and then deletes any chord that leaves only convex pieces. A chord deletion creates a nonconvex piece only if it creates an internal angle that is greater than 180 degrees. The decision of whether such an angle will be created can be made locally from the chords and edges surrounding the chord, in constant time. The result always contains no more than four times the minimum number of convex pieces.

I recommend using this heuristic unless it is critical for you to minimize the number of pieces. By experimenting with different triangulations and various deletion orders, you may be able to obtain somewhat better decompositions.

Dynamic programming may be used to find the absolute minimum number of diagonals used in the decomposition. The simplest implementation, which maintains the number of pieces for all $O(n^2)$ subpolygons split by a chord, runs in $O(n^4)$. Faster algorithms use fancier data structures, running in $O(n+r^2 \min(r^2, n))$ time, where r is the number of reflex vertices. An $O(n^3)$ algorithm that further reduces the number of pieces by adding interior vertices is cited below, although it is complex and presumably difficult to implement.

An alternate decomposition problem partitions polygons into *monotone* pieces. The vertices of a y-monotone polygon can be divided into two chains such that any horizontal line intersects either chain at most once.

Implementations: Many triangulation codes start by finding a trapezoidal or monotone decomposition of polygons. Further, a triangulation is a simple form of convex decomposition. Check out the codes in Section 17.3 (page 572) as a starting point.

CGAL (*www.cgal.org*) contains a polygon-partitioning library that includes (1) the Hertel-Mehlhorn heuristic for partitioning a polygon into convex pieces,

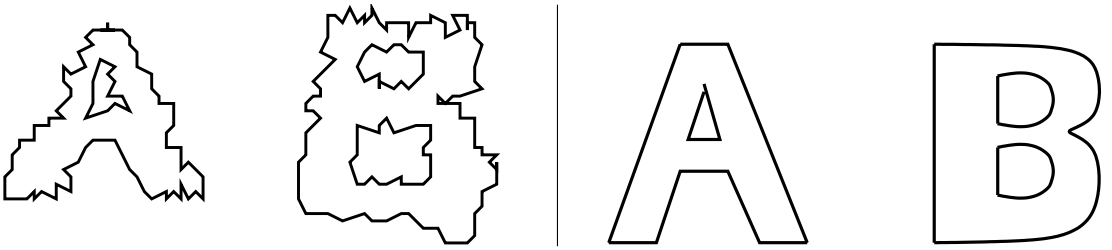
(2) finding a optimal convex partitioning using the $O(n^4)$ dynamic programming algorithm, and (3) an $O(n \log n)$ sweepline heuristic for partitioning into monotone polygons.

A triangulation code of particular relevance here is GEOMPACK—a suite of Fortran 77 codes by Barry Joe for 2- and 3-dimensional triangulation and convex decomposition problems. In particular, it does both Delaunay triangulation and convex decompositions of polygonal and polyhedral regions, as well as arbitrary-dimensional Delaunay triangulations.

Notes: Recent survey articles on polygon partitioning include [Kei00, OS04]. Keil and Sack [KS85] give an excellent survey on what is known about partitioning and covering polygons. Expositions on the Hertel-Mehlhorn heuristic [HM83] include [O'R01]. The $O(n+r^2 \min(r^2, n))$ dynamic programming algorithm for minimum convex decomposition using diagonals is due to Keil and Snoeyink [KS02]. The $O(r^3 + n)$ algorithm minimizing the number of convex pieces with Steiner points appears in [CD85]. Lien and Amato [LA06] provide an efficient heuristic for decomposing polygons with holes into "almost convex" polygons in $O(nr)$ time, with later work generalizing this to polyhedra.

Art gallery problems are an interesting topic related to polygon covering, where we seek to position the minimum number of guards in a given polygon such that every point in the interior of the polygon is watched by at least one guard. This corresponds to covering the polygon with a minimum number of star-shaped polygons. O'Rourke [O'R87] is a beautiful (although sadly out of print) book that presents the art gallery problem and its many variations.

Related Problems: Triangulation (see page 572), set cover (see page 621).



INPUT OUTPUT

17.12 Simplifying Polygons

Input description: A polygon or polyhedron p, with n vertices.

Problem description: Find a polygon or polyhedron p' containing only n' vertices, such that the shape of p' is as close as possible to p.

Discussion: Polygon simplification has two primary applications. The first involves cleaning up a noisy representation of a shape, perhaps obtained by scanning a picture of an object. Simplifying it can remove the noise and reconstruct the original object. The second involves data compression, where we seek to reduce detail on a large and complicated object yet leave it looking essentially the same. This can be a big win in computer graphics, where the smaller model might be significantly faster to render.

Several issues arise in shape simplification:

- *Do you want the convex hull?* – The simplest simplification is the convex hull of the object's vertices (see Section 17.2 (page 568)). The convex hull removes all internal concavities from the polygon. If you were simplifying a robot model for motion planning, this is almost certainly a good thing. But using the convex hull in an OCR system would be disastrous, because the concavities of characters provide most of the interesting features. An 'X' would be identical to an 'I', since both hulls are boxes. Another problem is that taking the convex hull of a convex polygon does nothing to simplify it further.

- *Am I allowed to insert or just delete points?* – The typical goal of simplification is to to represent the object as well as possible using a given number of vertices. The simplest approaches do local modifications to the boundary in order to reduce the vertex count. For example, if three consecutive vertices form a small-area triangle or define an extremely large angle, the center

vertex can be deleted and replaced with an edge without severely distorting the polygon.

Methods that only delete vertices quickly melt the shape into unrecognizability, however. More robust heuristics move vertices around to cover up the gaps that are created by deletions. Such "split-and-merge" heuristics can do a decent job, although nothing is guaranteed. Better results are likely by using the Douglas-Peucker algorithm, described next.

- *Must the resulting polygon be intersection-free?* – A serious drawback of incremental procedures is that they fail to ensure *simple* polygons, meaning they are without self-intersections. Thus "simplified" polygons may have ugly artifacts that may cause problems for subsequent routines. If simplicity is important, you should test all the line segments of your polygon for any pairwise intersections, as discussed in Section 17.8 (page 591).

  A polygon simplification approach that guarantees a simple approximation involves computing minimum-link paths. The *link distance* of a path between points s and t is the number of straight segments on the path. An as-the-crow-flies path has a link distance of one, while in general the link distance is one more than the number of turns on the path. The link distance between points s and t in a scene with obstacles is defined by the minimum link distance over all paths from s to t.

  The link distance approach "fattens" the boundary of the polygon by some acceptable error window ϵ (see Section 17.16 (page 617)) in order to construct a channel around the polygon. The minimum-link cycle in this channel represents the simplest polygon that never deviates from the original boundary by more than ϵ. An easy-to-compute approximation to link distance reduces it to breadth-first search, by placing a discrete set of possible turn points within the channel and connecting each pair of mutually visible points by an edge.

- *Are you given an image to clean up instead of a polygon to simplify?* – The conventional approach to cleaning up noise from a digital image is to take the Fourier transform of the image, filter out the high-frequency elements, and then take the inverse transform to recreate the image. See Section 13.11 (page 431) for details on the fast Fourier transform.

The Douglas-Puecker algorithm for shape simplification starts with a simple approximation and then refines it, instead of starting with a complicated polygon and trying to simplify it. Start by selecting two vertices v_1 and v_2 of polygon P, and propose the degenerate polygon v_1, v_2, v_1 as a simple approximation P'. Scan through each of the vertices of P, and select the one that is farthest from the corresponding edge of the polygon P'. Inserting this vertex adds the triangle to P' to minimize the maximum deviation from P. Points can be inserted until satisfactory results are achieved. This takes $O(kn)$ to insert k points when $|P| = n$.

Simplification becomes considerably more difficult in three dimensions. Indeed, it is NP-complete to find the minimum-size surface separating two polyhedra. Higher-dimensional analogies of the planar algorithms discussed here can be used to heuristically simplify polyhedra. See the Notes section.

Implementations: The Douglas-Peucker algorithm is readily implemented. Snoeyink provides a C implementation of his algorithm with efficient worst-case performance [HS94] at *http://www.cs.unc.edu/∼snoeyink/papers/DPsimp.arch*.

Simplification envelopes are a technique for automatically generating level-of-detail hierarchies for polygonal models. The user specifies a single error tolerance, and the maximum surface deviation of the simplified model from the original model, and a new, simplified model is generated. An implementation is available from *http://www.cs.unc.edu/∼geom/envelope.html*. This code preserves holes and prevents self-intersection.

QSlim is a quadric-based simplification algorithm that can produce high quality approximations of triangulated surfaces quite rapidly. It is available at *http://graphics.cs.uiuc.edu/∼garland/software.html*.

Yet another approach to polygonal simplification is based on simplifying and expanding the medial-axis transform of the polygon. The medial-axis transform (see Section 17.10 (page 598)) produces a skeleton of the polygon, which can be trimmed before inverting the transform to yield a simpler polygon. *Cocone* (*http://www.cse.ohio-state.edu/∼tamaldey/cocone.html*) constructs an approximate medial-axis transform of the polyhedral surface it interpolates from points in E^3. See [Dey06] for the theory behind *Cocone*. *Powercrust* [ACK01a, ACK01b] constructs a discrete approximation to the medial-axis transform, and then reconstructs the surface from this transform. When the point samples are sufficiently dense, the algorithm is guaranteed to produce a geometrically and topologically correct approximation to the surface. It is available at *http://www.cs.utexas.edu/users/amenta/powercrust/*.

CGAL (*www.cgal.org*) provides support for the most extreme polygon/polyhedral simplification, finding the smallest enclosing circle/sphere.

Notes: The Douglas-Peucker incremental refinement algorithm [DP73] is the basis for most shape simplification schemes, with faster implementations due to [HS94, HS98]. The link distance approach to polygon simplification is presented in [GHMS93]. Shape simplification problems become considerably more complex in three dimensions. Even finding the minimum-vertex convex polyhedron lying between two nested convex polyhedra is NP-complete [DJ92], although approximation algorithms are known [MS95b].

Heckbert and Garland [HG97] survey algorithms for shape simplification. Shape simplification using medial-axis transformations (see 17.10) are presented in [TH03].

Testing whether a polygon is simple can be performed in linear time, at least in theory, as a consequence of Chazelle's linear-time triangulation algorithm [Cha91].

Related Problems: Fourier transform (see page 431), convex hull (see page 568).

INPUT OUTPUT

17.13 Shape Similarity

Input description: Two polygonal shapes, P_1 and P_2.

Problem description: How similar are P_1 and P_2?

Discussion: Shape similarity is a problem that underlies much of pattern recognition. Consider a system for optical character recognition (OCR). We are given a library of shape models representing letters, and unknown shapes obtained by scanning a page. We seek to identify the unknown shapes by matching them to the most similar shape models.

Shape similarity is an inherently ill-defined problem, because what "similar" means is application dependent. Thus, no single algorithmic approach can solve all shape-matching problems. Whichever method you select, expect to spend a large chunk of time tweaking it to achieve maximum performance.

Among your possible approaches are

- *Hamming distance* – Assume that your two polygons have been overlaid one on top of the other. *Hamming distance* measures the area of symmetric difference between the two polygons—in other words, the area lying within one of the two polygons but not both of them. When two polygons are identical and properly aligned, the Hamming distance is zero. If the polygons differ only in a little noise at the boundary, then the Hamming distance of properly aligned polygons will be small.

  Computing the area of the symmetric difference reduces to finding the intersection or union of two polygons (discussed in Section 17.8 (page 591)) and then computing areas (discussed in Section 17.1). But the difficult part of

computing Hamming distance is finding the right alignment of the two polygons. This overlay problem is simplified in applications such as OCR because the characters are inherently aligned within lines on the page and are not free to rotate. Efficient algorithms for optimizing the overlap of convex polygons without rotation are cited below. Simple but reasonably effective heuristics are based on identifying reference landmarks on each polygon (such as the centroid, bounding box, or extremal vertices) and then matching a subset of these landmarks to define the alignment.

Hamming distance is particularly simple and efficient to compute on bit-mapped images, since after alignment all we do is sum the differences of the corresponding pixels. Although Hamming distance makes sense conceptually and can be simple to implement, it captures only a crude notion of shape and is likely to be ineffective in most applications.

- *Hausdorff distance* – An alternative distance metric is *Hausdorff distance*, which identifies the point on P_1 that is the maximum distance from P_2 and returns this distance. The Hausdorff distance is not symmetrical, for the tip of a long but thin protrusion from P_1 can imply a large Hausdorff distance P_1 to P_2, even though every point on P_2 is close to some point on P_1. A fattening of the entire boundary of one of the models (as is liable to happen with boundary noise) by a small amount may substantially increase the Hamming distance yet have little effect on the Hausdorff distance.

  Which is better, Hamming or Hausdorff? It depends upon your application. As with Hamming distance, computing the right alignment between the polygons can be difficult and time-consuming.

- *Comparing Skeletons* – A more powerful approach to shape similarity uses thinning (see Section 17.10 (page 598)) to extract a tree-like skeleton for each object. This skeleton captures many aspects of the original shape. The problem now reduces to comparing the shape of two such skeletons, using such features as the topology of the tree and the lengths/slopes of the edges. This comparison can be modeled as a form of subgraph isomorphism (see Section 16.9 (page 550)), with edges allowed to match whenever their lengths and slopes are sufficiently similar.

- *Support Vector Machines* – A final approach for pattern recognition/matching problems uses a learning-based technique such as neural networks or the more powerful *support vector machines*. These prove a reasonable approach to recognition problems when you have a lot of data to experiment with and no particular ideas of what to do with it. First, you must identify a set of easily computed features of the shape, such as area, number of sides, and number of holes. Based on these features, a black-box program (the support vector machine training algorithm) takes your training data and produces a classification function. This classification function accepts as input the values

of these features and returns a measure of what the shape is, or how close it is to a particular shape.

How good are the resulting classifiers? It depends upon the application. Like any ad hoc method, SVMs usually take a fair amount of tweaking and tuning to realize their full potential.

There is one caveat. If you don't know how/why black-box classifiers are making their decisions, you can't know when they will fail. An interesting case was a system built for the military to distinguish between images of cars and tanks. It performed very well on test images but disastrously in the field. Eventually, someone realized that the car images had been filmed on a sunnier day than the tanks, and the program was classifying solely on the presence of clouds in the background of the image!

Implementations: A Hausdorff-based image comparison implementation in C is available at *http://www.cs.cornell.edu/vision/hausdorff/hausmatch.html*. An alternate distance metric between polygons can be based on its angle-turning function [ACH+91]. An implementation in C of this turning function metric by Eugene K. Ressler is provided at *http://www.cs.sunysb.edu/∼algorith*.

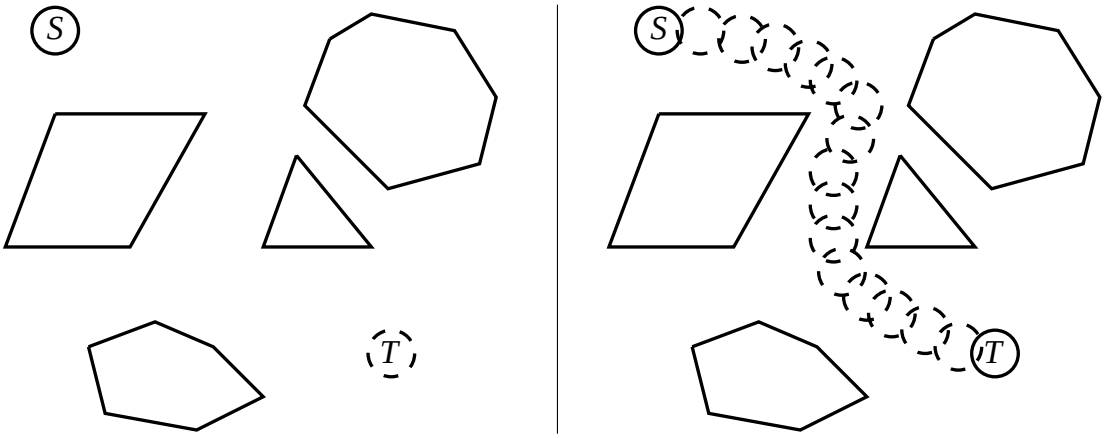
Several excellent support vector machine classifiers are available. These include the kernal-machine library (*http://www.terborg.net/research/kml/*), SVM^{light} (*http://svmlight.joachims.org/*) and the widely used and well-supported LIBSVM (*http://www.csie.ntu.edu.tw/∼cjlin/libsvm/*).

Notes: General books on pattern classification algorithms include [DHS00, JD88]. A wide variety of computational geometry approaches to shape similarity testing have been proposed, including [AMWW88, ACH+91, Ata84, AE83, BM89, OW85]. See the survey by Alt and Guibas [AG00].

The optimal alignment of n and m-vertex convex polygons subject to translation (but not rotation) can be computed in $O((n+m)\log(n+m))$ time [dBDK+98]. An approximation of the optimal overlap under translation and rotation is due to Ahn, et al. [ACP+07].

A linear-time algorithm for computing the Hausdorff distance between two convex polygons is given in [Ata83], with algorithms for the general case reported in [HK90].

Related Problems: Graph isomorphism (see page 550), thinning (see page 598).



INPUT OUTPUT

17.14 Motion Planning

Input description: A polygonal-shaped robot starting in a given position s in a room containing polygonal obstacles, and a goal position t.

Problem description: Find the shortest route taking s to t without intersecting any obstacles.

Discussion: That motion planning is a complex problem is obvious to anyone who has tried to move a large piece of furniture into a small apartment. It also arises in systems for molecular docking. Many drugs are small molecules that act by binding to a given target model. Identifying which binding sites are accessible to a candidate drug is clearly an instance of motion planning. Plotting paths for mobile robots is another canonical motion-planning application.

Finally, motion planning provides a tool for computer animation. Given the set of object models and where they appear in scenes s_1 and s_2, a motion planning algorithm can construct a short sequence of intermediate motions to transform s_1 to s_2. These motions can serve to fill in the intermediate scenes between s_1 and s_2, with such scene interpolation greatly reducing the workload on the animator.

Many factors govern the complexity of motion planning problems:

- *Is your robot a point?* – For point robots, motion planning becomes finding the shortest path from s to t around the obstacles. This is also known as geometric shortest path. The most readily implementable approach constructs the *visibility graph* of the polygonal obstacles, plus the points s and t. This

visibility graph has a vertex for each obstacle vertex and an edge between two obstacle vertices iff they "see" each other without being blocked by some obstacle edge.

The visibility graph can be constructed by testing each of the $\binom{n}{2}$ vertex-pair edge candidates for intersection against each of the n obstacle edges, although faster algorithms are known. Assign each edge of this visibility graph with weight equal to its length. Then the shortest path from s to t can be found using Dijkstra's shortest-path algorithm (see Section 15.4 (page 489)) in time bounded by the time required to construct the visibility graph.

- *What motions can your robot perform?* – Motion planning becomes considerably more difficult when the robot becomes a polygon instead of a point. Now all of the corridors that we use must be wide enough to permit the robot to pass through.

  The algorithmic complexity depends upon the number of *degrees of freedom* that the robot can use to move. Is it free to rotate as well as to translate? Does the robot have links that are free to bend or to rotate independently, as in an arm with a hand? Each degree of freedom corresponds to a dimension in the search space of possible configurations. Additional freedom makes it more likely that a short path exists from start to goal, although it also becomes harder to find this path.

- *Can you simplify the shape of your robot?* – Motion planning algorithms tend to be complex and time-consuming. Anything you can do to simplify your environment is a win. In particular, consider replacing your robot in an enclosing disk. If there is a start-to-goal path for this disk, it defines such a path for the robot inside of it. Furthermore, any orientation of a disk is equivalent to any other orientation, so rotation provides no help in finding a path. All movements can thus be limited to the simpler case of translation.

- *Are motions limited to translation only?* – When rotation is not allowed, the *expanded obstacles* approach can be used to reduce the problem of polygonal motion planning to the previously-resolved case of a point robot. Pick a reference point on the robot, and replace each obstacle by its Minkowski sum with the robot polygon (see Section 17.16 (page 617)). This creates a larger, fatter obstacle, defined by the shadow traced as the robot walks a loop around the object while maintaining contact with it. Finding a path from the initial reference position to the goal amidst these fattened obstacles defines a legal path for the polygonal robot in the original environment.

- *Are the obstacles known in advance?* – We have assumed that the robot starts out with a map of its environment. But this can't be true, say, in applications where the obstacles move. There are two approaches to solving motion-planning problems without a map. The first approach explores the

environment, building a map of what has been seen, and then uses this map to plan a path to the goal. A simpler strategy proceeds like a sightless man with a compass. Walk in the direction towards the goal until progress is blocked by an obstacle, and then trace a path along the obstacle until the robot is again free to proceed directly towards the goal. Unfortunately, this will fail in environments of sufficient complexity.

The most practical approach to general motion planning involves randomly sampling the *configuration space* of the robot. The configuration space defines the set of legal positions for the robot using one dimension for each degree of freedom. A planar robot capable of translation and rotation has three degrees of freedom, namely the x- and y-coordinates of a reference point on the robot and the angle θ relative to this point. Certain points in this space represent legal positions, while others intersect obstacles.

Construct a set of legal configuration-space points by random sampling. For each pair of points p_1 and p_2, decide whether there exists a direct, nonintersecting path between them. This defines a graph with vertices for each legal point and edges for each such traversable pair. Motion planning now reduces to finding a direct path from the initial/final position to some vertex in the graph, and then solving a shortest-path problem between the two vertices.

There are many ways to enhance this basic technique, such as adding additional vertices to regions of particular interest. Building such a road map provides a nice, clean approach to solving problems that would otherwise get very messy.

Implementations: The *Motion Planning Toolkit* (MPK) is a C++ library and toolkit for developing single- and multi-robot motion planners. It includes SBL, a fast single-query probabilistic roadmap path planner, and is available at *http://robotics.stanford.edu/∼mitul/mpk/*.

The University of North Carolina GAMMA group has produced several efficient collision detection libraries (not really motion planning) of which *SWIFT++* [EL01] is the most recent member of this family. It can detect intersection, compute approximate/exact distances between objects, and determine object-pair contacts in scenes composed of rigid polyhedral models. See *http://www.cs.unc.edu/∼geom/collide/* for pointers to all of these libraries.

The computational geometry library CGAL (*www.cgal.org*) contains many algorithms related to motion planning including visibility graph construction and Minkowski sums. O'Rourke [O'R01] gives a toy implementation of an algorithm to plot motion for a two-jointed robot arm in the plane. See Section 19.1.10 (page 662).

Notes: Latombe's book [Lat91] describes practical approaches to motion planning, including the random sampling method described above. Two other worthy books on motion planning are available freely on line, by LaValle [LaV06] (*http://planning.cs.uiuc.edu/*) and Laumond [Lau98] (*http://www.laas.fr/∼jpl/book.html*).

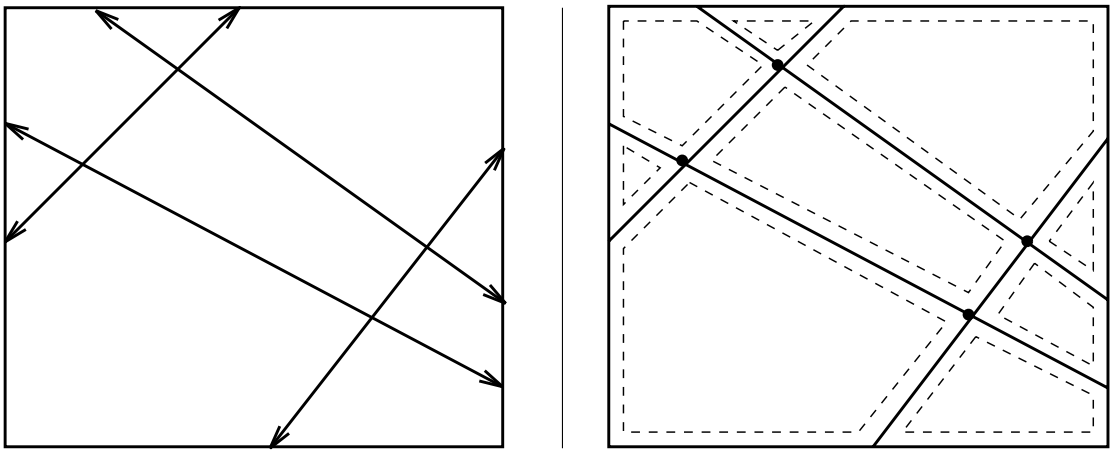
Motion planning was originally studied by Schwartz and Sharir as the "piano mover's problem." Their solution constructs the complete free space of robot positions that do not intersect obstacles, and then finds the shortest path within the proper connected component. These free space descriptions are very complicated, involving arrangements of higher-degree algebraic surfaces. The fundamental papers on the piano mover's problem appear in [HSS87], with [Sha04] a survey of current results.

The best general result for this free-space approach to motion planning is due to Canny [Can87], who showed that any problem with d degrees of freedom can be solved in $O(n^d \lg n)$, although faster algorithms exist for special cases of the general motion-planning problem. The expanded obstacle approach to motion planning is due to Lozano-Perez and Wesley [LPW79]. The heuristic, sightless man's approach to motion planning discussed previously has been studied by Lumelski [LS87].

The time complexity of algorithms based on the free-space approach to motion planning depends intimately on the combinatorial complexity of the arrangement of surfaces defining the free space. Algorithms for maintaining arrangements are presented in Section 17.15 (page 614). Davenport-Schinzel sequences often arise in the analysis of such arrangements. Sharir and Agarwal [SA95] provide a comprehensive treatment of Davenport-Schinzel sequences and their relevance to motion planning.

The visibility graph of n line segments with E pairs of visible vertices can be constructed in $O(n \lg n + E)$ time [GM91, PV96], which is optimal. Hershberger and Suri [HS99] have an $O(n \lg n)$ algorithm for finding shortest paths for point-robots with polygonal obstacles. Chew [Che85] provides an $O(n^2 \lg n)$ for finding shortest paths for a disk-robot in such a scene.

Related Problems: Shortest path (see page 489), Minkowski sum (see page 617).



INPUT OUTPUT

17.15 Maintaining Line Arrangements

Input description: A set of lines and line segments $l_1, \ldots, l_n$.

Problem description: What is the decomposition of the plane defined by $l_1, \ldots, l_n$?

Discussion: A fundamental problem in computational geometry is explicitly constructing the regions formed by the intersections of a set of n lines. Many problems reduce to constructing and analyzing such an arrangement of a specific set of lines. Examples include:

- *Degeneracy testing* – Given a set of n lines in the plane, do any three of them pass through the same point? Brute-force testing of all triples takes $O(n^3)$ time. Instead, we can construct the arrangement of the lines and then walk over each vertex and explicitly count its degree, all in quadratic time.
- *Satisfying the maximum number of linear constraints* – Suppose that we are given a set of n linear constraints, each of the form $y \leq a_i x + b_i$. Which point in the plane satisfies the largest number of them? Construct the arrangement of the lines. All points in any region or *cell* of this arrangement satisfy exactly the same set of constraints, so we need to test only one point per cell to find the global maximum.

Thinking of geometric problems in terms of features in an arrangement can be very useful in formulating algorithms. Unfortunately, it must be admitted that

arrangements are not as popular in practice as might be supposed. Primarily, this is because some depth of understanding is required to apply them correctly. The computational geometry library CGAL now provides a general and robust enough implementation to justify the effort to do so. Issues arising in arrangements include

- *What is the right way to construct a line arrangement?* – Algorithms for constructing arrangements are incremental. Begin with an arrangement of one or two lines. Subsequent lines are inserted into the arrangement one at a time, yielding larger and larger arrangements. To insert a new line, we start on the leftmost cell containing the line and walk over the arrangement to the right, moving from cell to neighboring cell and splitting into two pieces those cells that contain the new line.

- *How big will your arrangement be?* – A geometric fact called the *zone theorem* implies that the kth line inserted cuts through k cells of the arrangement, and further that $O(k)$ total edges form the boundary of these cells. This means that we can scan through each edge of every cell we encounter on our insertion walk, confident that only linear total work will be performed while inserting the line into the arrangement. Therefore, the total time to insert all n lines in constructing the full arrangement is $O(n^2)$.

- *What do you want to do with your arrangement?* – Given an arrangement and a query point, we are often interested in identifying which cell of the arrangement contains the point. This is the problem of point location, discussed in Section 17.7 (page 587). Given an arrangement of lines or line segments, we are often interested in computing all points of intersection of the lines. The problem of intersection detection is discussed in Section 17.8 (page 591).

- *Does your input consist of points instead of lines?* – Although lines and points seem to be different geometric objects, appearances can be misleading. Through the use of *duality transformations*, we can turn line L into point p and vice versa:

  $$L : y = 2ax - b \leftrightarrow p : (a, b)$$

  Duality is important because we can now apply line arrangements to point problems, often with surprising results.

  For example, suppose we are given a set of n points, and we want to know whether any three of them all lie on the same line. This sounds similar to the degeneracy testing problem discussed above. In fact it is *exactly the same*, with only the role of points and lines exchanged. We can dualize our points into lines as above, construct the arrangement, and then search for a vertex with three lines passing through it. The dual of this vertex defines the line on which the three initial vertices lie.

It often becomes useful to traverse each face of an existing arrangement exactly once. Such traversals are called *sweepline algorithms*, and are discussed in some detail in Section 17.8 (page 591). The basic procedure sorts the intersection points by x-coordinate and then walks from left to right while keeping track of all we have seen.

Implementations: CGAL (*www.cgal.org*) provides a generic and robust package for arrangements of curves (not just lines) in the plane. This should be the starting point for any serious project using arrangements.

A robust code for constructing and topologically sweeping an arrangement in C++ is provided at *http://www.cs.tufts.edu/research/geometry/other/sweep/*. An extension of topological sweep to deal with the visibility complex of a collection of pairwise disjoint convex planar sets has been provided in CGAL.

Arrange is a package for maintaining arrangements of polygons in either the plane or on the sphere. Polygons may be degenerate, and hence represent arrangements of lines. A randomized incremental construction algorithm is used, and efficient point location on the arrangement is supported. *Arrange* is written in C by Michael Goldwasser and is available from *http://euler.slu.edu/∼goldwasser/publications/*.

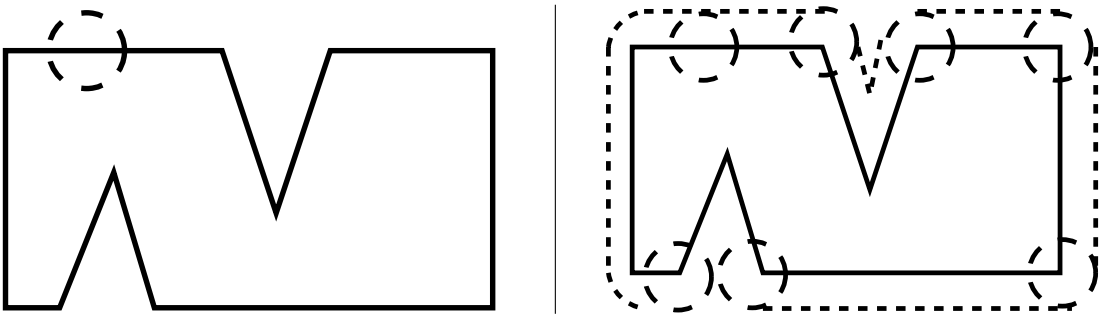
Notes: Edelsbrunner [Ede87] provides a comprehensive treatment of the combinatorial theory of arrangements, plus algorithms on arrangements with applications. It is an essential reference for anyone seriously interested in the subject. Recent surveys of combinatorial and algorithmic results include [AS00, Hal04]. Good expositions on constructing arrangements include [dBvKOS00, O'R01]. Implementation issues related to arrangements as implemented in CGAL are discussed in [FWH04, HH00].

Arrangements generalize naturally beyond two dimensions. Instead of lines, the space decomposition is defined by planes (or beyond 3-dimensions, *hyperplanes*). The zone theorem states that any arrangement of n d-dimensional hyperplanes has total complexity $O(n^d)$, and any single hyperplane intersects cells of complexity $O(n^{d-1})$. This provides the justification for the incremental construction algorithm for arrangements. Walking around the boundary of each cell to find the next cell that the hyperplane intersects takes time proportional to the number of cells created by inserting the hyperplane.

The history of the zone theorem has become somewhat muddled, because the original proofs were later found to be in error in higher dimensions. See [ESS93] for a discussion and a correct proof. The theory of Davenport-Schinzel sequences is intimately tied into the study of arrangements, which is presented in [SA95].

The naive algorithm for sweeping an arrangement of lines sorts the n^2 intersection points by x-coordinate and hence requires $O(n^2 \lg n)$ time. The *topological sweep* [EG89, EG91] eliminates the need to sort, and so traverses the arrangement in quadratic time. This algorithm is readily implementable and can be applied to speed up many sweepline algorithms. See [RSS02] for a robust implementation with experimental results.

Related Problems: Intersection detection (see page 591), point location (see page 587).



INPUT OUTPUT

17.16 Minkowski Sum

Input description: Point sets or polygons A and B, containing n and m vertices respectively.

Problem description: What is the convolution of A and B—i.e. , the Minkowski sum $A + B = \{x + y | x \in A, y \in B\}$?

Discussion: Minkowski sums are useful geometric operations that can *fatten* objects in appropriate ways. For example, a popular approach to motion planning for polygonal robots in a room with polygonal obstacles (see Section 17.14 (page 610)) fattens each of the obstacles by taking the Minkowski sum of them with the shape of the robot. This reduces the problem to the (more easily solved) case of point robots. Another application is in shape simplification (see Section 17.12 (page 604)). Here we fatten the boundary of an object to create a channel around it, and then let the minimum link path lying within this channel define the simplified shape. Finally, convolving an irregular object with a small circle will help smooth out the boundaries by eliminating minor nicks and cuts.

The definition of a Minkowski sum assumes that the polygons A and B have been positioned on a coordinate system:

$$A + B = \{x + y \mid x \in A, y \in B\}$$

where $x+y$ is the vector sum of two points. Thinking of this in terms of translation, the Minkowski sum is the union of all translations of A by a point defined within B. Issues arising in computing Minkowski sums include

- *Are your objects rasterized images or explicit polygons?* – The definition of Minkowski summation suggests a simple algorithm if A and B are rasterized images. Initialize a sufficiently large matrix of pixels by determining the size

of the convolution of the bounding boxes of A and B. For each pair of points in A and B, sum up their coordinates and darken the appropriate pixel. These algorithms get more complicated if an explicit polygonal representation of the Minkowski sum is needed.

- *Do you want to fatten your object by a fixed amount?* – The most common fattening operation expands a model M by a given tolerance t, known as *offsetting*. As shown in the figures above, this is accomplished by computing the Minkowski sum of M with a disk of radius t. The basic algorithms still work, although the offset is not a polygon. Its boundary is instead composed of circular arcs and line segments.

- *Are your objects convex or non-convex?* – The complexity of computing Minkowski sums depends in a serious way on the shape of the polygons. If both A and B are convex, the Minkowski sum can be found in $O(n+m)$ time by tracing the boundary of one polygon with another. If one of them is nonconvex, the *size* of the sum alone can be as large as $\Theta(nm)$. Even worse is when both A and B are nonconvex, in which case the *size* of the sum can be as large as $\Theta(n^2m^2)$. Minkowski sums of nonconvex polygons are often ugly in a majestic sort of way, with holes either created or destroyed in surprising fashion.

A straightforward approach to computing the Minkowski sum is based on triangulation and union. First, triangulate both polygons, then compute the Minkowski sum of each triangle of A against each triangle of B. The sum of a triangle against another triangle is easy to compute and is a special case of convex polygons, discussed below. The union of these $O(nm)$ convex polygons will be $A+B$. Algorithms for computing the union of polygons are based on plane sweep, as discussed in Section 17.8 (page 591).

Computing the Minkowski sum of two convex polygons is easier than the general case, because the sum will always be convex. For convex polygons it is easiest to slide A along the boundary of B and compute the sum edge by edge. Partitioning each polygon into a small number of convex pieces (see Section 17.11 (page 601)), and then unioning the Minkowski sum for each pair of pieces, will usually be much more efficient than working with two fully triangulated polygons.

Implementations: The CGAL (*www.cgal.org*) Minkowski sum package provides an efficient and robust code to find the Minkowski sums of two arbitrary polygons, as well as compute both exact and approximate offsets.

An implementation for computing the Minkowski sums of two convex polyhedra in $3D$ is described in [FH06] and available at *http://www.cs.tau.ac.il/∼efif/CD/*.

Notes: Good expositions on algorithms for Minkowski sums include [dBvKOS00, O'R01]. The fastest algorithms for various cases of Minkowski sums include [KOS91, Sha87].

The practical efficiency of Minkowski sum in the general case depends upon how the polygons are decomposed into convex pieces. The optimal solution is not necessarily the

partition into the fewest number of convex pieces. Agarwal et al. [AFH02] give a through study of decomposition methods for Minkowski sum.

The combinatorial complexity of the Minkowski sum of two convex polyhedra in three dimensions is completely resolved in [FHW07]. An implementation of Minkowski sum for such polyhedra is described in [FH06].

Kedem and Sharir [KS90] present an efficient algorithm for translational motion planning for polygonal robots, based on Minkowski sums.

Related Problems: Thinning (see page 598), motion planning (see page 610), simplifying polygons (see page 604).

18

Set and String Problems

Sets and strings both represent collections of objects—the difference is whether order matters. Sets are collections of symbols whose order is assumed to carry no significance, while strings are defined by the sequence or arrangement of symbols.

The assumption of a fixed order makes it possible to solve string problems much more efficiently than set problems, through techniques such as dynamic programming and advanced data structures like suffix trees. The interest in and importance of string-processing algorithms have been increasing due to bioinformatics, Web searches, and other text-processing applications. Recent books on string algorithms include:

- *Gusfield* [Gus97] – To my taste, this remains is the best introduction to string algorithms. It contains a thorough discussion on suffix trees, with clear and innovative formulations of classical exact string-matching algorithms.
- *Crochemore, Hancart, and Lecroq* [CHL07] – A comprehensive treatment of string algorithms, written by a true leader in the field. Translated from the French, but clear and accessible.
- *Navarro and Raffinot* [NR07] – A concise but practical and implementation-oriented treatment of pattern-matching algorithms, with particularly thorough treatment of bit-parallel approaches.
- *Crochemore and Rytter* [CR03] – A survey of specialized topics in string algorithmics emphasizing theory.

Theoreticians working in string algorithmics sometimes refer to their field as *Stringology*. The annual *Combinatorial Pattern Matching* (CPM) conference is the primary venue devoted to both practical and theoretical aspects of string algorithmics and related areas.

S.S. Skiena, *The Algorithm Design Manual*, 2nd ed., DOI: 10.1007/978-1-84800-070-4_18,
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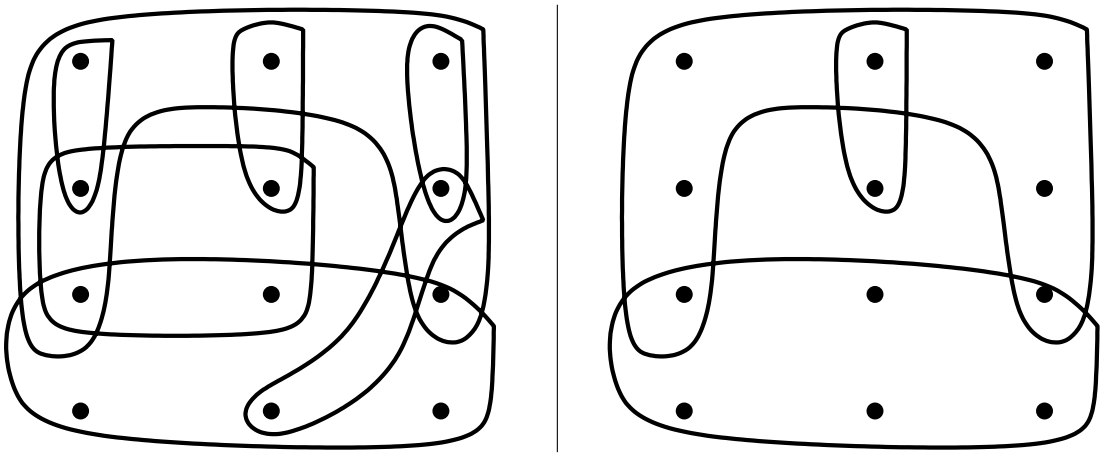


INPUT OUTPUT

18.1 Set Cover

Input description: A collection of subsets $S = \{S_1, \ldots, S_m\}$ of the universal set $U = \{1, \ldots, n\}$.

Problem description: What is the smallest subset T of S whose union equals the universal set—i.e. , $\cup_{i=1}^{|T|} T_i = U$?

Discussion: Set cover arises when you try to efficiently acquire items that have been packaged in a fixed set of lots. You seek a collection of at least one of each distinct type of item, while buying as few lots as possible. Finding *a* set cover is easy, because you can always buy one of each possible lot. However, identifying a small set cover let you do the same job for less money. Set cover provided a natural formulation of the Lotto ticket optimization problem discussed in Section 1.6 (page 23). There we seek to buy the smallest number of tickets needed to cover all of a given set of combinations.

Boolean logic minimization is another interesting application of set cover. We are given a particular Boolean function of k variables, which describes whether the desired output is 0 or 1 for each of the 2^k possible input vectors. We seek the simplest circuit that exactly implements this function. One approach is to find a disjunctive normal form (DNF) formula on the variables and their complements, such as $x_1\bar{x}_2 + \bar{x}_1\bar{x}_2$. We could build one "and" term for each input vector and then "or" them all together, but we might save considerably by factoring out common subsets of variables. Given a set of feasible "and" terms, each of which covers a

subset of the vectors we need, we seek to "or" together the smallest number of terms that realize the function. This is exactly the set cover problem.

There are several variations of set cover problems to be aware of:

- *Are you allowed to cover elements more than once?* – The distinction here is between *set cover* and *set packing*, which is discussed in Section 18.2 (page 625). We should take advantage of the freedom to cover elements multiple times if we have it, as it usually results in a smaller covering.

- *Are your sets derived from the edges or vertices of a graph?* – Set cover is a very general problem, and includes several useful graph problems as special cases. Suppose instead that you seek the smallest set of edges in a graph that will cover each vertex at least once. The solution is the maximum *matching* in the graph (see Section 15.6 (page 498)), plus arbitrary edges to cover any unmatched vertices. Now suppose instead that you seek the smallest set of vertices that cover each edge at least once. This is the *vertex cover* problem, discussed in Section 16.3 (page 530).

  It is instructive to show how to model vertex cover as an instance of set cover. Let the universal set U correspond to the set of edges $\{e_1, \ldots, e_m\}$. Construct n subsets, with S_i consisting of the edges incident on vertex v_i. Although vertex cover is just an instance of set cover in disguise, you should take advantage of the superior heuristics that exist for the more restricted vertex cover problem.

- *Do your subsets contain only two elements each?* – You are in luck if all of your subsets have at most two elements each. This special case can be solved efficiently to optimality because it reduces to finding a maximum matching in a graph. Unfortunately, the problem becomes NP-complete as soon as your subsets have three elements each.

- *Do you want to cover elements with sets, or sets with elements?* – In the *hitting set* problem, we seek a small number of items that together represent each subset in a given population. Hitting set is illustrated in Figure 18.1. The input is identical to set cover, but instead we seek the smallest subset of elements $T \subset U$ such that each subset S_i contains at least one element of T. Thus, $S_i \cap T \neq \emptyset$ for all $1 \leq i \leq m$. Suppose we desire a small Congress with at least one representative for each ethnic group. If each ethnic group is defined by a subset of people, the minimum hitting set gives the smallest possible politically correct Congress.

  Hitting set is *dual* to set cover, meaning that it is exactly the same problem in disguise. Replace each element of U by a set of the names of the subsets that contain it. Now S and U have exchanged roles, for we seek a set of subsets from U to cover all the elements of S. This is exactly set cover, so we can use any set cover code to solve hitting set after performing this simple translation. See Figure 18.1 for an example.

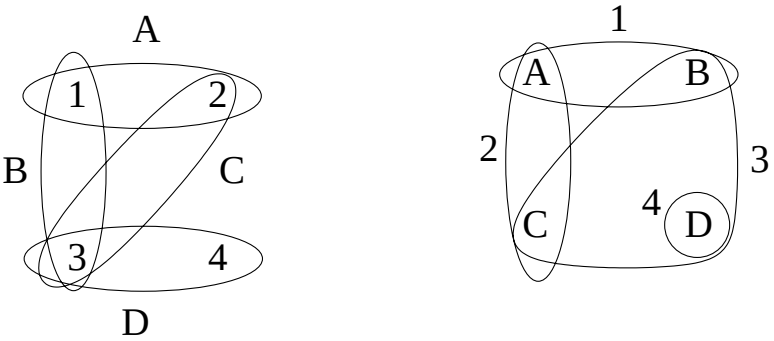


Figure 18.1: A hitting set instance optimally solved by selecting elements 1 and 3 or 2 and 3 (l). This problem converted to a dual set cover instance optimally solved by selecting subsets 1 and 3 or 2 and 4 (r).

Set cover must be at least as hard as vertex cover, so it is also NP-complete. In fact, it is somewhat harder. Approximation algorithms do no worse than twice optimal for vertex cover, but the best approximation algorithm for set cover is $\Theta(\lg n)$ times optimal.

Greedy is the most natural and effective heuristic for set cover. Begin by selecting the largest subset for the cover, and then delete all its elements from the universal set. We add the subset containing the largest number of remaining uncovered elements repeatedly until all are covered. This heuristic always gives a set cover using at most $\ln n$ times as many sets as optimal. In practice it usually does a lot better.

The simplest implementation of the greedy heuristic sweeps through the entire input instance of m subsets for each greedy step. However, by using such data structures as linked lists and a bounded-height priority queue (see Section 12.2 (page 373)), the greedy heuristic can be implemented in $O(S)$ time, where $S = \cup_{i=1}^{m} |S_i|$ is the size of the input representation.

It pays to check whether or not there exist elements that exist in only a few subsets—ideally only one. If so, we should select the biggest subsets containing these elements at the very beginning. We must take such a subset eventually, and they carry along other elements that we might have paid extra to cover if we wait until later.

Simulated annealing is likely to produce somewhat better set covers than these simple heuristics. Backtracking can be used to guarantee you an optimal solution, but it is usually not worth the computational expense.

An alternate and more powerful approach rests on the integer programming formulation of set cover. Let the integer 0-1 variable s_i denote whether subset S_i is selected for a given cover. Each universal set element x adds the constraint

$$\sum_{x \in S_i} s_i \geq 1$$

to ensure that it is covered by at least one selected subset. The minimum set cover satisfies all constraints while minimizing $\sum_i s_i$. This integer program can be easily generalized to weighted set cover (allowing nonuniform costs for different subsets. Relaxing this to a linear program (i.e. , allowing $0 \leq s_i \leq 1$ instead of constricting each variable to be either 0 or 1) allows efficient and effective heuristics using rounding techniques.

Implementations: Both the greedy heuristic and the above ILP formulation are sufficiently simple in their respective worlds that one has to implement them from scratch.

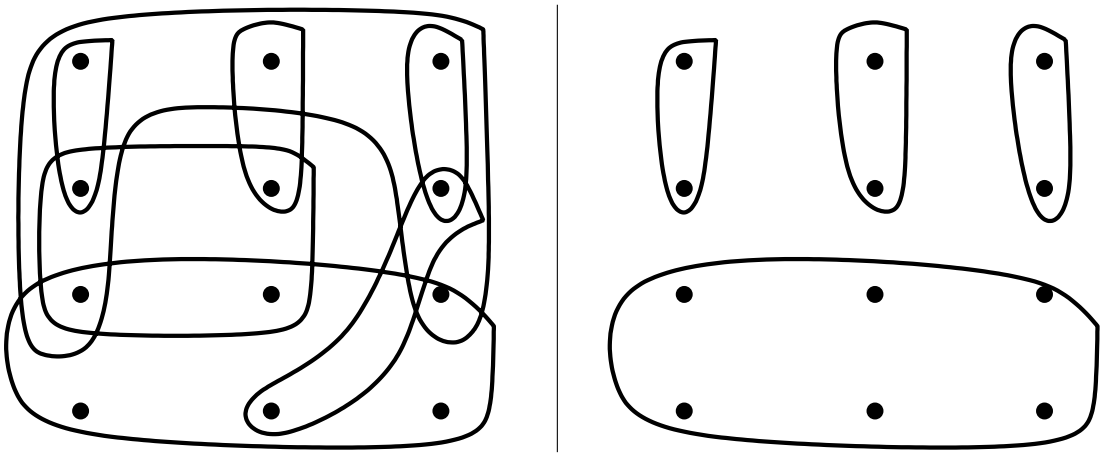
Pascal implementations of an exhaustive search algorithm for set packing, as well as heuristics for set cover, appear in [SDK83]. See Section 19.1.10 (page 662).

SYMPHONY is a mixed-integer linear programming solver that includes a set partitioning solver. It is available at *http://branchandcut.org/SPP/*

Notes: An old but classic survey article on set cover is [BP76], with more recent approximation and complexity analysis surveyed in [Pas97]. See [CFT99, CFT00] for extensive computational studies of integer programming-based set cover heuristics and exact algorithms. An excellent exposition on algorithms and reduction rules for set cover is presented in [SDK83].

Good expositions of the greedy heuristic for set cover include [CLRS01, Hoc96]. An example demonstrating that the greedy heuristic for set cover can be as bad as $\lg n$ is presented in [Joh74, PS98]. This is not a defect of the heuristic. Indeed, it is provably hard to approximate set cover to within an approximation factor better than $(1 - o(1)) \ln n$ [Fei98].

Related Problems: Matching (see page 498), vertex cover (see page 530), set packing (see page 625).



INPUT OUTPUT

18.2 Set Packing

Input description: A set of subsets $S = \{S_1, \ldots, S_m\}$ of the universal set $U = \{1, \ldots, n\}$.

Problem description: Select (an ideally small) collection of mutually disjoint subsets from S whose union is the universal set.

Discussion: Set-packing problems arise in applications where we have strong constraints on what is an allowable partition. The key feature of packing problems is that no elements are permitted to be covered by more than one selected subset.

Some flavor of this is captured by the independent set problem in graphs, discussed in Section 16.2 (page 528). There we seek a large subset of vertices from graph G such that each edge is adjacent to at most one of the selected vertices. To model this as set packing, let the universal set consist of all edges of G, and subset S_i consist of all edges incident on vertex v_i. Finally, define an additional singleton set for each edge. Any set packing defines a set of vertices with no edge in common—in other words, an independent set. The singleton sets are used to pick up any edges not covered by the selected vertices.

Scheduling airline flight crews is another application of set packing. Each airplane in the fleet needs to have a crew assigned to it, consisting of a pilot, copilot, and navigator. There are constraints on the composition of possible crews, based on their training to fly different types of aircraft, personality conflicts, and work schedules. Given all possible crew and plane combinations, each represented by a subset of items, we need an assignment such that each plane and each person is

in exactly one chosen combination. After all, the same person cannot be on two different planes simultaneously, and every plane needs a crew. We need a perfect packing given the subset constraints.

Set packing is used here to represent several problems on sets, all of which are NP-complete:

- *Must every element appear in exactly one selected subset?* – In the *exact cover* problem, we seek some collection of subsets such that each element is covered exactly once. The airplane scheduling problem above has the flavor of exact covering, since every plane and crew has to be employed.

  Unfortunately, exact cover puts us in a situation similar to that of Hamiltonian cycle in graphs. If we really *must* cover all the elements exactly once, and this existential problem is NP-complete, then all we can do is exponential search. The cost will be prohibitive unless we happen to stumble upon a solution quickly.

- *Does each element have its own singleton set?* – Things will be far better if we can be content with a partial solution, say by including each element of U as a singleton subset of S. Thus, we can expand any set packing into an exact cover by mopping up the unpacked elements of U with singleton sets. Now our problem is reduced to finding a minimum-cardinality set packing, which can be attacked via heuristics.

- *What is the penalty for covering elements twice?* – In set cover (see Section 18.1 (page 621)), there is no penalty for elements existing in many selected subsets. In exact cover, any such violation is forbidden. For many applications, the truth lies somewhere in between. Such problems can be approached by charging the greedy heuristic more to select a subset that contains previously covered elements.

The right heuristics for set packing are greedy, and similar to those of set cover (see Section 18.1 (page 621)). If we seek a packing with many (few) sets, then we repeatedly select the smallest (largest) subset, delete all subsets from S that clash with it, and repeat. As usual, augmenting this approach with some exhaustive search or randomization (in the form of simulated annealing) is likely to yield better packings at the cost of additional computation.

An alternate and more powerful approach rests on an integer programming formulation akin to that of set cover. Let the integer 0-1 variable s_i denote whether subset S_i is selected for a given cover. Each universal set element x adds the constraint

$$\sum_{x \in S_i} s_i = 1$$

to ensure that it is covered by *exactly* one selected subset. Minimizing or maximizing $\sum_i s_i$ while respecting these constraints enables us modulate the desired number of sets in the cover.

Implementations: Since set cover is a more popular and more tractable problem than set packing, it might be easier to find an appropriate implementation to solve the cover problem. Such implementations discussed in Section 18.1 (page 621) should be readily modifiable to support certain packing constraints.

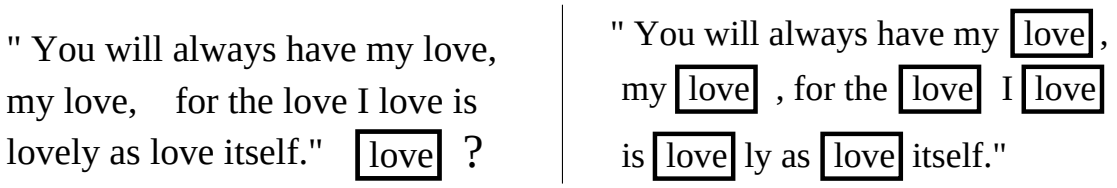
Pascal implementations of an exhaustive search algorithm for set packing, as well as heuristics for set cover, appear in [SDK83]. See Section 19.1.10 (page 662) for details on FTP-ing these codes.

SYMPHONY is a mixed-integer linear programming solver that includes a set partitioning solver. It is available at *http://branchandcut.org/SPP/*.

Notes: Survey articles on set packing include [BP76, Pas97]. Bidding strategies for combinatorial auctions typically reduce to solving set-packing problems, as described in [dVV03].

Set-packing relaxations for integer programs are presented in [BW00]. An excellent exposition on algorithms and reduction rules for set packing is presented in [SDK83], including the airplane scheduling application discussed previously.

Related Problems: Independent set (see page 528), set cover (see page 621).



18.3 String Matching

Input description: A text string t of length n. A pattern string p of length m.

Problem description: Find the first (or all) instances of pattern p in the text.

Discussion: String matching arises in almost all text-processing applications. Every text editor contains a mechanism to search the current document for arbitrary strings. Pattern-matching programming languages such as Perl and Python derive much of their power from their built-in string matching primitives, making it easy to fashion programs that filter and modify text. Spelling checkers scan an input text for words appearing in the dictionary and reject any strings that do not match.

Several issues arise in identifying the right string matching algorithm for a given application:

- *Are your search patterns and/or texts short?* – If your strings are sufficiently short and your queries sufficiently infrequent, the simple $O(mn)$-time search algorithm will suffice. For each possible starting position $1 \leq i \leq n - m + 1$, it tests whether the m characters starting from the ith position of the text are identical to the pattern. An implementation of this algorithm (in C) is given in Section 2.5.3 (page 43).

  For very short patterns (say $m \leq 5$), you can't hope to beat this simple algorithm by much, so you shouldn't try. Further, we expect much better than $O(mn)$ behavior for typical strings, because we advance the pattern the instant we observe a text/pattern mismatch, Indeed, the trivial algorithm *usually* runs in linear time. But the worst case certainly can occur, as with pattern $p = a^m$ and text $t = (a^{m-1}b)^{n/m}$.

- *What about longer texts and patterns?* – String matching can in fact be performed in worst-case linear time. Observe that we need not begin the search from scratch on finding a character mismatch, since the pattern prefix and text must exactly match up to the point of mismatch. Given a long partial

match ending at position i, we jump ahead to the first character position in the pattern/text that can provide new information about the text in position $i + 1$. The Knuth-Morris-Pratt algorithm preprocesses the search pattern to construct such a jump table efficiently. The details are tricky to get correct, but the resulting algorithm yields short, simple programs.

- *Do I expect to find the pattern or not?* – The Boyer-Moore algorithm matches the pattern against the text from right to left, and can avoid looking at large chunks of text on a mismatch. Suppose the pattern is *abracadabra*, and the eleventh character of the text is x. This pattern cannot match in any of the first eleven starting positions of the text, and so the next necessary position to test is the 22nd character. If we get very lucky, only n/m characters need ever be tested. The Boyer-Moore algorithm involves two sets of jump tables in the case of a mismatch: one based on pattern matched so far, the other on the text character seen in the mismatch.

  Although somewhat more complicated than Knuth-Morris-Pratt, it is worth it in practice for patterns of length $m > 5$, unless the pattern is expected to occur many times in the text. Its worst-case performance is $O(n + rm)$, where r is the number of occurrences of p in t.

- *Will you perform multiple queries on the same text?* – Suppose you are building a program to repeatedly search a particular text database, such as the Bible. Since the text remains fixed, it pays to build a data structure to speed up search queries. The suffix tree and suffix array data structures, discussed in Section 12.3 (page 377), are the right tools for the job.

- *Will you search many texts using the same patterns?* – Suppose you are building a program to screen out dirty words from a text stream. Here, the set of patterns remains stable, while the search texts are free to change. In such applications, we may need to find all occurrences of any of k different patterns where k can be quite large.

  Performing a linear-time scan for each pattern yields an $O(k(m + n))$ algorithm. If k is large, a better solution builds a single finite automaton that recognizes all of these patterns and returns to the appropriate start state on any character mismatch. The Aho-Corasick algorithm builds such an automaton in linear time. Space savings can be achieved by optimizing the pattern recognition automaton, as discussed in Section 18.7 (page 646). This approach was used in the original version of *fgrep*.

  Sometimes multiple patterns are specified not as a list of strings, but concisely as a regular expression. For example, the regular expression $a(a + b + c)^*a$ matches any string on (a, b, c) that begins and ends with a distinct a. The best way to test whether an input string is described by a given regular expression R constructs the finite automaton equivalent to R and then simulates

the machine on the string. Again, see Section 18.7 (page 646) for details on constructing automata from regular expressions.

When the patterns are specified by context-free grammars instead of regular expressions, the problem becomes one of parsing, discussed in Section 8.6 (page 298).

- *What if our text or pattern contains a spelling error?* – The algorithms discussed here work only for exact string matching. If you want to allow some tolerance for spelling errors, your problem becomes *approximate string matching*, which is thoroughly discussed in Section 18.4 (page 631).

Implementations: Strmat is a collection of C programs implementing exact pattern matching algorithms in association with [Gus97], including several variants of the KMP and Boyer-Moore algorithms. It is available at *http://www.cs.ucdavis.edu/~gusfield/strmat.html*.

SPARE Parts [WC04a] is a C++ string pattern recognition toolkit that provides production-quality implementations of all major variants of the classical string-matching algorithms for single patterns (both Knuth-Morris-Pratt and Boyer-Moore) and multiple patterns (both Aho-Corasick and Commentz-Walter). It is available at *http://www.fastar.org/*.

Several versions of the general regular expression pattern matcher (grep) are readily available. GNU *grep* found at *http://directory.fsf.org/project/grep/*, and supersedes variants such as *egrep* and *fgrep*. GNU *grep* uses a fast lazy-state deterministic matcher hybridized with a Boyer-Moore search for fixed strings.

The Boost string algorithms library provides C++ routines for basic operations on strings, including search. See *http://www.boost.org/doc/html/string_algo.html*.

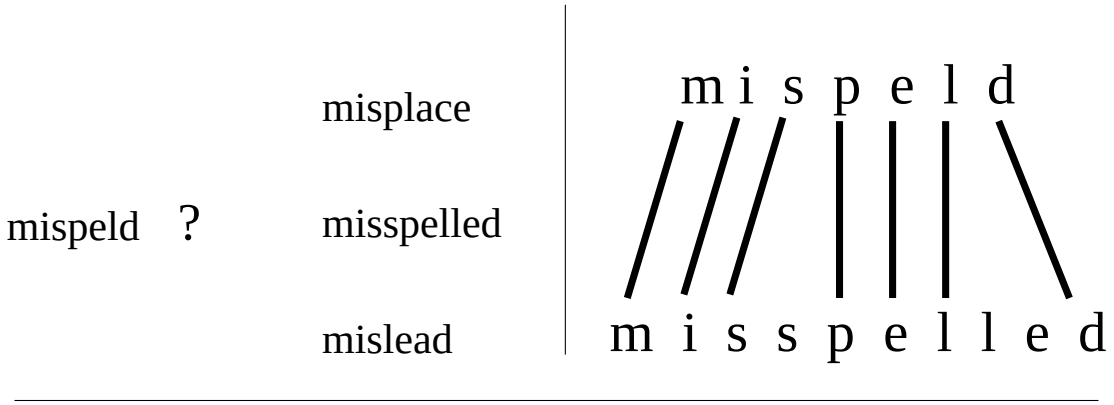
Notes: All books on string algorithms contain thorough discussions of exact string matching, including [CHL07, NR07, Gus97]. Good expositions on the Boyer-Moore [BM77] and Knuth-Morris-Pratt algorithms [KMP77] include [BvG99, CLRS01, Man89]. The history of string matching algorithms is somewhat checkered because several published proofs were incorrect or incomplete. See [Gus97] for clarification.

Aho [Aho90] provides a good survey on algorithms for pattern matching in strings, particularly where the patterns are regular expressions instead of strings. The Aho-Corasick algorithm for multiple patterns is described in [AC75].

Empirical comparisons of string matching algorithms include [DB86, Hor80, Lec95, dVS82]. Which algorithm performs best depends upon the properties of the strings and the size of the alphabet. For long patterns and texts, I recommend that you use the best implementation of Boyer-Moore that you can find.

The Karp-Rabin algorithm [KR87] uses a hash function to perform string matching in linear expected time. Its worst-case time remains quadratic, and its performance in practice appears somewhat worse than the character comparison methods described above. This algorithm is presented in Section 3.7.2 (page 91).

Related Problems: Suffix trees (see page 377), approximate string matching (see page 631).



18.4 Approximate String Matching

Input description: A text string t and a pattern string p.

Problem description: What is the minimum-cost way to transform t to p using insertions, deletions, and substitutions?

Discussion: Approximate string matching is a fundamental problem because we live in an error-prone world. Spelling correction programs must be able to identify the closest match for any text string not found in a dictionary. By supporting efficient sequence similarity (homology) searches on large databases of DNA sequences, the computer program BLAST has revolutionized the study of molecular biology. Suppose you were interested in a particular gene in man, and discovered that it is similar to the hemoglobin gene in rats. Likely this new gene also produces hemoglobin, and any differences are the result of genetic mutations during evolution.

I once encountered approximate string matching when evaluating the performance of an optical character-recognition system. We needed to compare the answers produced by our system on a test document with the correct results. To improve our system, we needed to identify (1) which letters were getting misidentified and (2) gibberish when the program found letters that didn't exist. The solution was to do an alignment between the two texts. Insertions and deletions corresponded to gibberish, while substitutions signaled errors in our recognizer. This same principle is used in file difference programs, which identify the lines that have changed between two versions of a file.

When no errors are permitted, our problem reduces to exact string matching, which is presented in Section 18.3 (page 628). Here, we restrict our discussion to matching with errors.

Dynamic programming provides the basic approach to approximate string matching. Let $D[i,j]$ denote the cost of editing the first i characters of the pattern string p into the first j characters of the text t. The recurrence follows because we must have done *something* with the tail characters p_i and t_j. Our only options are matching / substituting one for the other, deleting p_i, or inserting a match for t_j. Thus, $D[i,j]$ is the minimum of the costs of these possibilities:

1. If $p_i = t_j$ then $D[i-1,j-1]$ else $D[i-1,j-1]$ + substitution cost.
2. $D[i-1,j]$ + deletion cost of p_i.
3. $D[i,j-1]$ + deletion cost of t_j.

A general implementation in C and more complete discussion appears in Section 8.2 (page 280). Several issues remain before we can make full use of this recurrence:

- *Do I match the pattern against the full text, or against a substring?* – The boundary conditions of this recurrence distinguishes between algorithms for string matching and substring matching. Suppose we want to align the full pattern against the full text. Then the cost of $D[i,0]$ must be that of deleting the first i characters of the pattern, so $D[i,0] = i$. Similarly, $D[0,j] = j$.

  Now suppose that the pattern can occur anywhere within the text. The proper cost of $D[0,j]$ is now 0, since there should be no penalty for starting the alignment in the jth position of the text. The cost of $D[i,0]$ remains i, because the only way to match the first i pattern characters with nothing is to delete all of them. The cost of the best substring pattern match against the text will be given by $\min_{k=1}^{n} D[m,k]$.

- *How should I select the substitution and insertion/deletion costs?* – The basic algorithm can be easily modified to use different costs for insertion, deletion, and the substitutions of specific pairs of characters. Which costs you should use depend on what you are planning to do with the alignment.

  The most common cost assignment charges the same for insertion, deletion, or substitution. Charging a substitution cost of more than insertion + deletion ensures that substitutions never get performed, since it will always be cheaper to edit both characters out of the string. If we just have insertion and deletion to work with, the problem reduces to *longest common subsequence*, discussed in Section 18.8 (page 650). It often pays to tweak the edit distance costs and study the resulting alignments until you find the best parameters for the job.

- *How do I find the actual alignment of the strings?* – As thus far described, the recurrence only gives the cost of the optimal string/pattern alignment, not the sequence of editing operations to achieve it. To obtain such a transcript, we can work backwards from the complete cost matrix D. We had to come from one of $D[m-1,n]$ (pattern deletion/text insertion), $D[m,n-1]$

(text deletion/pattern insertion), or $D[m-1, n-1]$ (substitution/match) to get to cell $D[m, n]$. The option which was chosen can be reconstructed from these costs and the given characters p_m and t_n. By continuing to work backwards to the previous cell, we can reconstruct the entire alignment. Again, an implementation in C appears in Section 8.2 (page 280).

- *What if the two strings are very similar to each other?* – The dynamic programming algorithm finds a shortest path across an $m \times n$ grid, where the cost of each edge depends upon which operation it represents. To seek an alignment involving a combination of at most d insertions, deletions, and substitutions, we need only traverse the band of $O(dn)$ cells within a distance d of the central diagonal. If no low-cost alignment exists within this band, then no low-cost alignment can exist in the full cost matrix.

  Another idea we can use is *filtration*, quickly eliminating the parts of the string where there is no hope of finding the pattern. Carve the m-length pattern into $d+1$ pieces. If there is a match with at most d differences, then at least one of these pieces must be an exact match in the optimal alignment. Thus, we can identify all possible approximate match points by conducting an exact multi-pattern search on the pieces, and then evaluate only the possible candidates more carefully.

- *Is your pattern short or long?* – A recent approach to string-matching exploits the fact that modern computers can do operations on (say) 64-bit words in a single gulp. This is long enough to hold eight 8-bit ASCII characters, providing motivation to design *bit-parallel algorithms*, which do more than one comparison with each operation.

  The basic idea is quite clever. Construct a bit-mask B_α for each letter α of the alphabet, such that ith-bit $B_\alpha[i] = 1$ iff the ith character of the pattern is α. Now suppose you have a match bit-vector M_j for position j in the text string, such that $M_j[i] = 1$ iff the first i bits of the pattern exactly match the $(j-i+1)$st through jth character of the text. We can find *all* the bits of M_{j+1} using just two operations by (1) shifting M_j one bit to the right, and then (2) doing a bitwise AND with B_α, where α is the character in position $j+1$ of the text.

  The *agrep* program, discussed below, uses such a bit-parallel algorithm generalized to approximate matching. Such algorithms are easy to program and many times faster than dynamic programming.

- *How can I minimize the required storage?* – The quadratic space used to store the dynamic programming table is usually a more serious problem than its running time. Fortunately, only $O(\min(m, n))$ space is needed to compute $D[m, n]$. We need only maintain two active rows (or columns) of the matrix to compute the final value. The entire matrix will be required only if we need to reconstruct the actual sequence alignment.

We can use Hirschberg's clever recursive algorithm to efficiently recover the optimal alignment in linear space. During one pass of the linear-space algorithm above to compute $D[m, n]$, we identify which middle-element cell $D[m/2, x]$ was used to optimize $D[m, n]$. This reduces our problem to finding the best paths from $D[1, 1]$ to $D[m/2, x]$ and from $D[m/2, x]$ to $D[m/2, n]$, both of which can be solved recursively. Each time we remove half of the matrix elements from consideration, so the total time remains $O(mn)$. This linear-space algorithm proves to be a big win in practice on long strings, although it is somewhat more difficult to program.

- *Should I score long runs of indels differently?* – Many string matching applications look more kindly on alignments where insertions/deletions are bunched in a small number of runs or gaps. Deleting a word from a text should presumably cost less than a similar number of scattered single-character deletions, because the word represents a single (albeit substantial) edit operation.

  String matching with *gap penalties* provides a way to properly account for such operations. Typically, we assign a cost of $A + Bt$ for each indel of t consecutive characters, where A is the cost of starting the gap and B is the per-character deletion cost. If A is large relative to B, the alignment has incentive to create relatively few runs of deletions.

  String matching under such *affine* gap penalties can be done in the same quadratic time as regular edit distance. We will use separate insertion and deletion recurrences E and F to encode the cost of being in gap mode, meaning we have already paid the cost of initiating the gap:

$$V(i, j) = \max(E(i, j), F(i, j), G(i, j))$$

$$G(i, j) = V(i - 1, j - 1) + match(i, j)$$

$$E(i, j) = \max(E(i, j - 1), V(i, j - 1) - A) - B$$

$$F(i, j) = \max(F(i - 1, j), V(i - 1, j) - A) - B$$

  With a constant amount of work per cell, this algorithm takes $O(mn)$ time, same as without gap costs.

- *Does similarity mean strings that sound alike?* – Other models of approximate pattern matching become more appropriate for certain applications. Particularly interesting is *Soundex*, a hashing scheme that attempts to pair up English words that sound alike. This can be useful in testing whether two names that have been spelled differently are likely to be the same. For example, my last name is often spelled "Skina", "Skinnia", "Schiena", and occasionally "Skiena." All of these hash to the same Soundex code, *S25*.

The algorithm drops vowels and silent letters, removes doubled letters, and then assigns the remaining letters numbers from the following classes: *BFPV* gets a 1, *CGJKQSXZ* gets a 2, *DT* gets a 3, *L* gets a 4, *MN* gets a 5, and *R* gets a 6. The code starts with the first letter and contains at most three digits. Although this sounds very hokey, experience shows that it works reasonably well. Experience indeed: Soundex has been used since the 1920's.

Implementations: Several excellent software tools are available for approximate pattern matching. Manber and Wu's *agrep* [WM92a, WM92b] (approximate general regular expression pattern matcher) is a tool supporting text search with spelling errors. A recent version is available from *http://www.tgries.de/agrep/*. Navarro's *nrgrep* [Nav01b] combines bit-parallelism and filtration, resulting in running times that are more constant than *agrep*, although not always faster. It is available at *http://www.dcc.uchile.cl/~gnavarro/software/*.

TRE is a general regular-expression matching library for exact and approximate matching, which is more general than *agrep*. The worst-case complexity is $O(nm^2)$, where m is the list of the regular expressions involved. *TRE* is available at *http://laurikari.net/tre/*.

Wikipedia gives programs for computing edit (Levenshtein) distance in a dizzying array of languages (including Ada, C++, Emacs Lisp, Io, JavaScript, Java, PHP, Python, Ruby VB, and C#) Check it out at:

http://en.wikibooks.org/wiki/Algorithm_implementation/Strings/Levenshtein_distance

Notes: There have been many recent advances in approximate string matching, particularly in bit-parallel algorithms. Navarro and Raffinot [NR07] is the best reference on these recent techniques, which are also treated in other recent books on string algorithmics [CHL07, Gus97]. String matching with gap penalties is particularly well treated in [Gus97].

The basic dynamic programming alignment algorithm is attributed to [WF74], although it is apparently folklore. The wide range of applications for approximate string matching was made apparent in Sankoff and Kruskal's book [SK99], which remains a useful historical reference for the problem. Surveys on approximate pattern matching include [HD80, Nav01a]. The edit distance between two strings is sometimes referred to as the *Levenshtein distance*. Expositions of Hirschberg's linear-space algorithm [Hir75] include [CR03, Gus97].

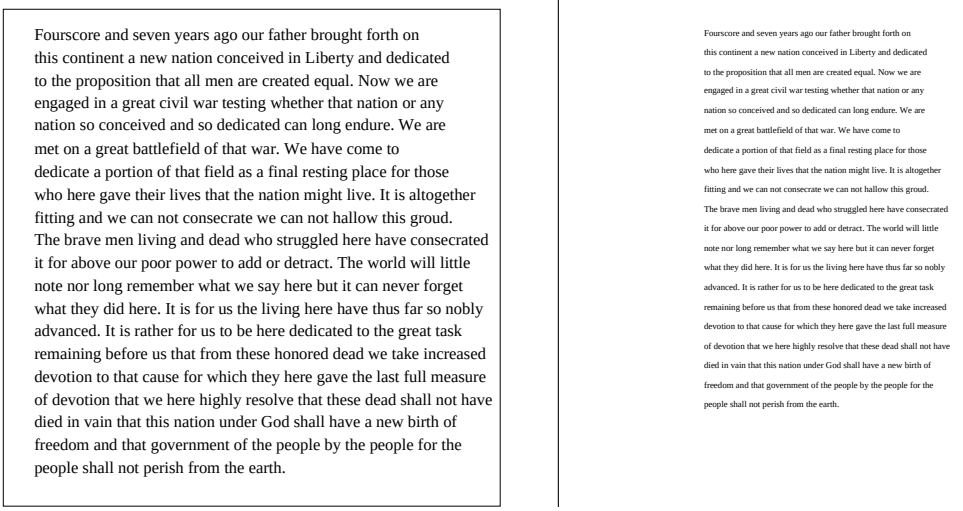
Masek and Paterson [MP80] compute the edit distance between m- and n-length strings in time $O(mn/\log(\min\{m,n\}))$ for constant-sized alphabets, using ideas from the four Russians algorithm for Boolean matrix multiplication [ADKF70].

The shortest path formulation leads to a variety of algorithms that are good when the edit distance is small, including an $O(n \lg n + d^2)$ algorithm due to Myers [Mye86] and an $O(dn)$ algorithm due to Landau and Vishkin [LV88]. Longest increasing subsequence can be done in $O(n \lg n)$ time [HS77], as presented in [Man89].

Bit-parallel algorithms for approximate matching include Myers's [Mye99b] algorithm for approximate matching in $O(mn/w)$ time, where w is the number of bits in the computer word. Experimental studies of bit-parallel algorithms include [FN04, HFN05, NR00].

Soundex was invented and patented by M. K. Odell and R. C. Russell. Expositions on Soundex include [BR95, Knu98]. Metaphone is a recent attempt to improve on Soundex [BR95, Par90]. See [LMS06] for an application of such phonetic hashing techniques to the problem entity name unification.

Related Problems: String matching (see page 628), longest common substring (see page 650).



INPUT OUTPUT

18.5 Text Compression

Input description: A text string S.

Problem description: Create a shorter text string S' such that S can be correctly reconstructed from S'.

Discussion: Secondary storage devices fill up quickly on every computer system, even though their capacity continues to double every year. Decreasing storage prices only seem to have increased interest in data compression, probably because there is more data to compress than ever before. *Data compression* is the algorithmic problem of finding space-efficient encodings for a given data file. The rise of computer networks provided a new mission for data compression, that of increasing the effective network bandwidth by reducing the number of bits before transmission.

People seem to *like* inventing ad hoc data-compression methods for their particular application. Sometimes these outperform general methods, but often they don't. Several issues arise in selecting the right compression algorithm:

- *Must we recover the exact input text after compression? – Lossy* versus *lossless* encoding is the primary issue in data compression. Document storage applications typically demand lossless encodings, as users become disturbed

whenever their data files are altered. Fidelity is not such an issue in image or video compression, because the presence of small artifacts are imperceptible to the viewer. Significantly greater compression ratios can be obtained using lossy compression, which is why most image/video/audio compression algorithms exploit this freedom.

- *Can I simplify my data before I compress it?* – The most effective way to free space on a disk is to delete files you don't need. Likewise, any preprocessing you can do to reduce the information content of a file pays off later in better compression. Can we eliminate redundant white space from the file? Might the document be converted entirely to uppercase characters, or have formatting information removed?

  A particularly interesting simplification results from applying the *Burrows-Wheeler transform* to the input string. This transform sorts all n cyclic shifts of the n character input, and then reports the last character of each shift. As an example, the cyclic shifts of $ABAB$ are $ABAB$, $BABA$, $ABAB$, and $BABA$. After sorting, these become $ABAB$, $ABAB$, $BABA$, and $BABA$. Reading the last character of each of these strings yields the transform result: $BBAA$.

  Provided the last character of the input string is unique (e.g., end-of-string), this transform is perfectly reversible to the original input! The Burrows-Wheeler string is typically 10-15% more compressible than the original text, because repeated words turn into blocks of repeated characters. Further, this transform can be computed in linear time.

- *Does it matter whether the algorithm is patented?* – Certain data compression algorithms have been patented—most notoriously the LZW variation of the Lempel-Ziv algorithm discussed below. Mercifully, this patent has now expired, although legal battles are still being fought over JPEG. Typically there are unrestricted variations of any compression algorithm that perform about as well as the patented variant.

- *How do I compress image data* – The simplest lossless compression algorithm for image data is *run-length coding*. Here we replace runs of identical pixel values with a single instance of the pixel and an integer giving the length of the run. This works well on binary images with large contiguous regions of similar pixels, like scanned text. It performs badly on images with many quantization levels and random noise. Correctly selecting (1) the number of bits to allocate to the count field, and (2) the right traversal order to reduce a two-dimensional image into a stream of pixels, has a surprisingly important impact on compression.

  For serious audio/image/video compression applications, I recommend that you use a popular lossy coding method and not fool around with implementing it yourself. JPEG is the standard high-performance image compression

method, while MPEG is designed to exploit the frame-to-frame coherence of video.

- *Must compression run in real time?* – Fast decompression is often more important than fast compression. A YouTube video is compressed only once, but decompressed every time someone plays it. In contrast, an operating system that increases effective disk capacity by automatically compressing files will need a symmetric algorithm with fast compression times, as well.

Literally dozens of text compression algorithms are available, but they can be classified into two distinct approaches. *Static algorithms*, such as Huffman codes, build a single coding table by analyzing the entire document. *Adaptive algorithms*, such as Lempel-Ziv, build a coding table on the fly that adapts to the local character distribution of the document. Adaptive algorithms usually prove to be the correct answer:

- *Huffman codes* – Huffman codes replace each alphabet symbol by a variable-length code string. Using eight bits-per-symbol to encode English text is wasteful, since certain characters (such as "e") occur far more frequently than others (such as "q"). Huffman codes assign "e" a short code word, and "q" a longer one to compress text.

  Huffman codes can be constructed using a greedy algorithm. Sort the symbols in increasing order by frequency. We merge the two least-frequently used symbols x and y into a new symbol xy, whose frequency is the sum of the frequencies of its two child symbols. Replacing x and y by xy leaves a smaller set of symbols. We now repeat this operation $n - 1$ times until all symbols have been merged. These merging operations define a rooted binary tree, with the original alphabet symbols as leaves. The left or right choices on the root-to-leaf path define the bits of the binary code word for each symbol. Priority queues can efficiently maintain the symbols by frequency during construction, yielding Huffman codes in $O(n \lg n)$ time.

  Huffman codes are popular but have three disadvantages. Two passes must be made over the document on encoding, first to build the coding table, and then to actually encode the document. The coding table must be explicitly stored with the document to decode it, which eats into any space savings on short documents. Finally, Huffman codes only exploit nonuniform symbol distributions, while adaptive algorithms can recognize the higher-order redundancies such as in *0101010101...*.

- *Lempel-Ziv algorithms* – Lempel-Ziv algorithms (including the popular LZW variant) compress text by building a coding table on the fly as we read the document. The coding table changes at every position in the text. A clever protocol ensures that the encoder and decoder are both always working with the exact same code table, so no information is lost.

> Lempel-Ziv algorithms build coding tables of frequent substrings, which can get arbitrarily long. Thus they can exploit often-used syllables, words, and phrases to build better encodings. It adapts to local changes in the text distribution, which is important because many documents exhibit significant locality of reference.
>
> The truly amazing thing about the Lempel-Ziv algorithm is how robust it is on different types of data. It is quite difficult to beat Lempel-Ziv by using an application-specific algorithm. My recommendation is not to try. If you can eliminate application-specific redundancies with a simple preprocessing step, go ahead and do it. But don't waste much time fooling around. You are unlikely to get significantly better text compression than with *gzip* or some other popular program, and you might well do worse.

Implementations: Perhaps the most popular text compression program is *gzip*, which implements a public domain variation of the Lempel-Ziv algorithm. It is distributed under the GNU software license and can be obtained from *http://www.gzip.org*.

There is a natural tradeoff between compression ratio and compression time. Another choice is *bzip2*, which uses the Burrows-Wheeler transform. It produces tighter encodings than *gzip* at somewhat greater cost in running time. Going to the extreme, other compression algorithms devote enormous run times to squeeze every bit out of a file. Representative programs of this genre are collected at *http://www.cs.fit.edu/~mmahoney/compression/*.

Reasonably authoritative comparisons of compression programs are presented at *http://www.maximumcompression.com/*, including links to all available software.

Notes: A large number of books on data compression are available. Recent and comprehensive books include Sayood [Say05] and Salomon [Sal06]. Also recommended is the older book by Bell, Cleary, and Witten [BCW90]. Surveys on text compression algorithms include [CL98].

Good expositions on Huffman codes [Huf52] include [AHU83, CLRS01, Man89]. The Lempel-Ziv algorithm and variants are described in [Wel84, ZL78]. The Burrows-Wheeler transform was introduced in [BW94].

The annual IEEE Data Compression Conference (*http://www.cs.brandeis.edu/~dcc/*) is the primary research venue in this field. This is a mature technical area where most current work is shooting for fairly marginal improvements, particularly in the case of text compression. More encouragingly, we note that the conference is held annually at a world-class ski resort in Utah.

Related Problems: Shortest common superstring (see page 654), cryptography (see page 641).

The magic words are Squeamish Ossifrage.	I5&AE<&UA9VEC'=0 <F1s"F%R92!3<75E96UI<V V@*3W-S:69R86=E+@K_

INPUT OUTPUT

18.6 Cryptography

Input description: A plaintext message T or encrypted text E, and a key k.

Problem description: Encode T (decode E) using k giving E (T).

Discussion: Cryptography has grown substantially in importance as computer networks make confidential documents more vulnerable to prying eyes. Cryptography increases security by making messages difficult to read even if they fall into the wrong hands. Although the discipline of cryptography is at least two thousand years old, its algorithmic and mathematical foundations have only recently solidified to the point where provably secure cryptosystems can be envisioned.

Cryptographic ideas and applications go beyond the commonly known concepts of "encryption" and "authentication." The field now includes such important mathematical constructs such as cryptographic hashes, digital signatures, and useful primitive protocols that provide associated security assurances.

There are three classes of cryptosystems everyone should be aware of:

- *Caesar shifts* – The oldest ciphers involve mapping each character of the alphabet to a different letter. The weakest such ciphers rotate the alphabet by some fixed number of characters (often 13), and thus have only 26 possible keys. Better is to use an arbitrary permutation of the letters, giving 26! possible keys. Even so, such systems can be easily attacked by counting the frequency of each symbol and exploiting the fact that "e" occurs more often than "z". While there are variants that will make this more difficult to break, none will be as secure as AES or RSA.

- *Block Shuffle Ciphers* – This class of algorithms repeatedly shuffle the bits of your text as governed by the key. The classic example of such a cipher is the *Data Encryption Standard* (DES). Although approved as a Federal Information Processing Standard in 1976, its 56-bit key length is now considered too short for applications requiring substantial levels of security. Indeed, a special purpose machine named "Deep Crack" demonstrated that it is possible to decrypt messages without a key in less than a day. As of May 19,

2005, *DES* has been officially withdrawn as a federal standard, replaced by the stronger *Advanced Encryption Standard* (AES).

However, a simple variant called *triple DES* permits an effective key length of 112 bits by using three rounds of DES with two 56-bit keys. In particular, first encrypt with key1, then *decrypt* with key2, before finally encrypting with key1. There is a mathematical reason for using three rounds instead of two; the encrypt-decrypt-encrypt pattern is used so that the scheme is equivalent to single DES when $key1 = key2$. This is enough to keep "Deep Crack" at bay. Indeed, *triple DES* has recently been approved by the National Institute of Standards and Technology (NIST) for sensitive government information through the year 2030.

- *Public Key Cryptography* – If you fear bad guys reading your messages, you should be afraid to tell anyone else the key needed to decrypt them. Public-key systems use different keys to encode and decode messages. Since the encoding key is of no help in decoding, it can be made public at no risk to security. This solution to the key distribution problem is literally its key to success.

  RSA is the classic example of a public key cryptosystem, named after its inventors Rivest, Shamir, and Adelman. The security of RSA is based on the relative computational complexities of factoring and primality testing (see Section 13.8 (page 420)). Encoding is (relatively) fast because it relies on primality testing to construct the key, while the hardness of decryption follows from that of factoring. Still, RSA is slow relative to other cryptosystems—roughly 100 to 1,000 times slower than DES.

The critical issue in selecting a cryptosystem is identifying your paranoia level—i.e. , deciding how much security you need. Who are you trying to stop from reading your stuff: your grandmother, local thieves, the Mafia, or the NSA? If you can use an accepted implementation of AES or RSA, you should feel pretty safe against anybody, at least for now. Increasing computer power often lays waste to cryptosystems surprisingly quickly; recall that DES lived less than 30 years as a strong system. Be sure to use the longest possible keys and keep abreast of algorithmic development if you are a planning long-term storage of criminal material.

That said, I will confess that I use DES to encrypt my final exam each semester. It proved more than sufficient the time an ambitious student broke into my office looking for it. The story would have been different had the NSA had been breaking in, but it is important to understand that *the most serious security holes are human, not algorithmic*. Ensuring that your password is long enough, hard to guess, and not written down is far more important than obsessing about the encryption algorithm.

Most symmetric key encryption mechanisms are harder to crack than public key ones for the same key size. This means one can get away with much shorter key lengths for symmetric key than for public key encryption. NIST and RSA Labs

both provide schedules of recommended key sizes for secure encryption, and as of this writing they recommend 80-bit symmetric keys as equivalent to 1024-bit asymetric keys. This difference helps explain why symmetric key algorithms are typically orders of magnitude faster than public key algorithms.

Simple ciphers like the Caesar shift are fun and easy to program. For this reason, it is healthy to use them for applications needing only a casual level of security (such as hiding the punchlines of jokes). Since they are easy to break, they should never be used for serious security applications.

Another thing you should *never* do is try to develop your own novel cryptosystem. The security of triple DES and RSA is accepted because these systems have survived many years of public scrutiny. In this time, many other cryptosystems have been proposed, proven vulnerable to attack, and then abandoned. This is not a field for amateurs. If you are charged with implementing a cryptosystem, carefully study a respected program such as PGP to see how they handle issues such as key selection and key distribution. Any cryptosystem is as strong as its weakest link.

Certain other problems related to cryptography arise often in practice:

- *How can I validate the integrity of data against random corruption?* – There is often a need to validate that transmitted data is identical to that which has been received. One solution is for the receiver to transmit the data back to the source and have the original sender confirm that the two texts are identical. This fails when the exact inverse of an error is made in the retransmission, but a more serious problem is that your available bandwidth is cut in half with such a scheme.

  A more efficient method uses a *checksum*, a simple mathematical function that hashes a long text down to a simple number or digit. We then transmit the checksum along with the text. The checksum can be recomputed on the receiving end and bells set off if the computed checksum is not identical to what was received. The simplest checksum scheme just adds up the byte or character values and takes the sum modulo of some constant, say $2^8 = 256$. Unfortunately, an error transposing two or more characters would go undetected under such a scheme, since addition is commutative.

  Cyclic-redundancy check (CRC) provides a more powerful method for computing checksums that is used in most communications systems and internally in computers to validate disk drive transfers. These codes compute the remainder in the ratio of two polynomials, the numerator of which is a function of the input text. The design of these polynomials involves considerable mathematical sophistication, but ensures that all reasonable errors are detected. The details of efficient computation are sufficiently complicated that we recommend that you start from an existing implementation, described below.

- *How can I validate the integrity of data against deliberate corruption?* – CRC is good at detecting random errors, but not malicious changes to a document. *Cryptographic hashing functions* such as MD5 and SHA-256 are (in principle) easy to compute for a document but hard to invert. This means that given a particular hash code value x, it is difficult to construct a document d such that $H(d) = x$. The property makes them valuable for digital signatures and other applications.

- *How can I prove that a file has not been changed?* – If I send you a contract in electronic form, what is to stop you from editing the file and then claiming that your version was what we had really agreed to? I need a way to prove that any modification to a document is fraudulent. *Digital signatures* are a cryptographic way for me to stamp my document as genuine.

  Given a file, I can compute a checksum for it, and then encrypt this checksum using my own private key. I send you the file and the encrypted checksum. You can now edit the file, but to fool the judge you must also edit the encrypted checksum such that it can be decrypted to yield the correct checksum. With a suitably good checksum function, designing a file that yields the same checksum becomes an insurmountable problem. For full security, we need a trusted third party to authenticate the timestamp and associate the private key with me.

- *How can I restrict access to copyrighted material?* – An important emerging application for cryptography is digital rights management for audio and video. A key issue here is speed of decryption, as it must keep up with data transmission or retrieval in real time. Such *stream ciphers* usually involve efficiently generating a stream of pseudorandom bits, say using a shift-register generator. The exclusive-or of these bits with the data stream gives the encrypted sequence. The original data is recovered by exclusive-oring the result with the same stream of pseudorandom bits.

  High-speed cryptosystems have proven to be relatively easy to break. The state-of-the-art solution to this problem involves erecting laws like the Digital Millennium Copyright Act to make it illegal to try to break them.

Implementations: *Nettle* is a comprehensive low-level cryptographic library in C. Cryptographic hash functions include MD5 and SHA-256. Block ciphers include DES, AES, and some more recently developed codes. An implementation of RSA is also provided. *Nettle* is available at *http://www.lysator.liu.se/∼nisse/nettle*.

A comprehensive overview of cryptographic algorithms with assessments of strength is available at *http://www.cryptolounge.org/wiki/Category:Algorithm*. See *http://csrc.nist.gov/groups/ST/toolkit* for related cryptographic resources provided by NIST.

Crypto++ is a large C++ class library of cryptographic schemes, including all we have mentioned in this section. It is available at *http://www.cryptopp.com/*.

Many popular open source utilities employ serious cryptography, and serve as good models of current practice. *GnuPG*, an open source version of PGP, is available at *http://www.gnupg.org/*. *OpenSSL*, for authenticating access to computer systems, is available at *http://www.openssl.org/*.

The *Boost CRC Library* provides multiple implementations of cyclic redundancy check algorithms. It is available at *http://www.boost.org/libs/crc/*.

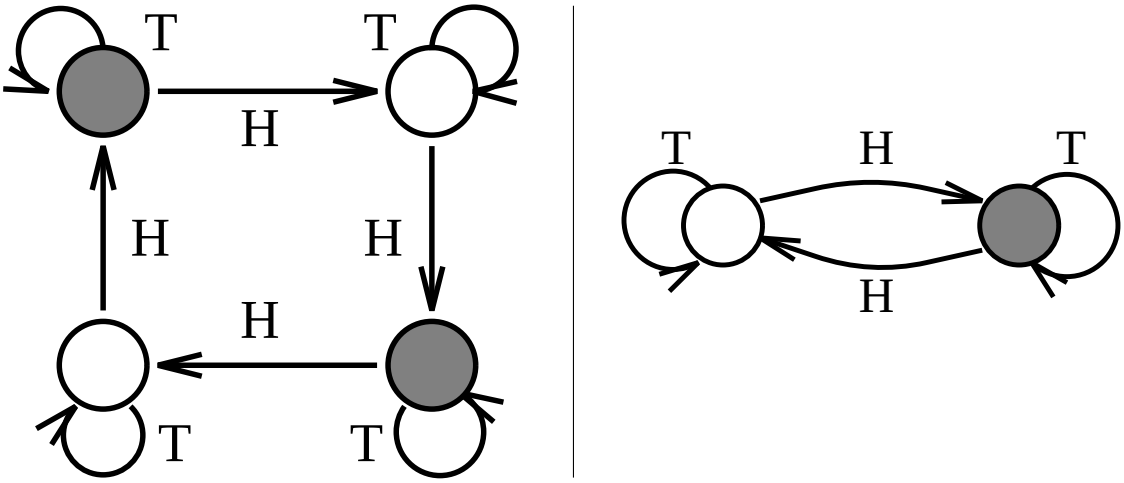
Notes: The *Handbook of Applied Cryptography* [MOV96] provides technical surveys of all aspects of cryptography, and has been generously made available online at *http://www.cacr.math.uwaterloo.ca/hac/*. Schneier [Sch96] provides a thorough overview of different cryptographic algorithms, with [FS03] as perhaps a better introduction. Kahn [Kah67] presents the fascinating history of cryptography from ancient times to 1967 and is particularly noteworthy in light of the secretive nature of the subject.

Expositions on the RSA algorithm [RSA78] include [CLRS01]. The RSA Laboratories home page *http://www.rsa.com/rsalabs/* is very informative.

Of course, the NSA (National Security Agency) is the place to go to learn the real state of the art in cryptography. The history of DES is well presented in [Sch96]. Particularly controversial was the decision by the NSA to limit key length to 56 bits.

MD5 [Riv92] is the hashing function used by PGP to compute digital signatures. Expositions include [Sch96, Sta06]. Serious problems with the security of MD5 have recently been exposed [WY05]. The SHA family of hash functions appears more secure, particularly SHA-256 and SHA-512.

Related Problems: Factoring and primality testing (see page 420), text compression (see page 637)).



INPUT OUTPUT

18.7 Finite State Machine Minimization

Input description: A deterministic finite automaton M.

Problem description: Create the smallest deterministic finite automaton M' such that M' behaves identically to M.

Discussion: Constructing and minimizing finite state machines arises repeatedly in software and hardware design applications. Finite state machines are very useful for specifying and recognizing patterns. Modern programming languages such as Java and Python provide built-in support for *regular expressions*, a particularly natural way of defining automata. Control systems and compilers often use finite state machines to encode the current state and possible associated actions/transitions. Minimizing the size of these automata reduces both the storage and execution costs of dealing with such machines.

Finite state machines are defined by directed graphs. Each vertex represents a state, and each character-labeled edge defines a transition from one state to another on receipt of the given alphabet symbol. The automata shown analyzes a sequence of coin tosses, with dark states signifying that an even number of heads have been observed. Such automata can be represented using any graph data structure (see Section 12.4 (page 381)), or by an $n \times |\Sigma|$ *transition matrix* where $|\Sigma|$ is the size of the alphabet.

Finite state machines are often used to specify search patterns in the guise of regular expressions, which are patterns formed by and-ing, or-ing, and looping

over smaller regular expressions. For example, the regular expression $a(a+b+c)^*a$ matches any string on (a, b, c) that begins and ends with distinct as. The best way to test whether a string s is recognized by a given regular expression R constructs the finite automaton equivalent to R, and then simulates this machine on S. See Section 18.3 (page 628) for alternative approaches to string matching.

We consider three different problems on finite automata:

- *Minimizing deterministic finite state machines* – Transition matrices for finite automata become prohibitively large for sophisticated machines, thus fueling the need for tighter encodings. The most direct approach is to eliminate redundant states in the automaton. As the example above illustrates, automata of widely varying sizes can compute the same function.

  Algorithms for minimizing the number of states in a deterministic finite automaton (DFA) appear in any book on automata theory. The basic approach partitions the states into gross equivalence classes and then refines the partition. Initially, the states are partitioned into accepting, rejecting, and other classes. The transitions from each node now branch to a given class on a given symbol. Whenever two states s, t from the same class C branch to elements of different classes, the class C must be partitioned into two subclasses, one containing s, the other containing t.

  This algorithm makes a sweep though all the classes looking for a new partition, and repeats the process from scratch if it finds one. This yields an $O(n^2)$ algorithm, since at most $n-1$ sweeps need ever be performed. The final equivalence classes correspond to the states in the minimum automaton. In fact, a more efficient $O(n \log n)$ algorithm is known. Implementations are cited below.

- *Constructing deterministic machines from nondeterministic machines* – DFAs are simple to work with, because the machine is always in exactly one state at any given time. *Nondeterministic automata* (NFAs) can be in multiple states at a time, so their current "state" represents a subset of all possible machine states.

  In fact, any NFA can be mechanically converted to an equivalent DFA, which can then be minimized as above. However, converting an NFA to a DFA might cause an exponential blowup in the number of states, which perversely might then be eliminated when minimizing the DFA. This exponential blowup makes most NFA minimization problems PSPACE-hard, which is even worse than NP-complete.

  The proofs of equivalence between NFAs, DFAs, and regular expressions are elementary enough to be covered in undergraduate automata theory classes. However, they are surprisingly nasty to actually code. Implementations are discussed below.

- *Constructing machines from regular expressions* – There are two approaches for translating a regular expression to an equivalent finite automaton. The difference is whether the output automaton will be a nondeterministic or deterministic machine. NFAs are easier to construct but less efficient to simulate.

  The nondeterministic construction uses ϵ-moves, which are optional transitions that require no input to fire. On reaching a state with an ϵ-move, we must assume that the machine can be in either state. Using ϵ-moves, it is straightforward to construct an automaton from a depth-first traversal of the parse tree of the regular expression. This machine will have $O(m)$ states, if m is the length of the regular expression. Furthermore, simulating this machine on a string of length n takes $O(mn)$ time, since we need consider each state/prefix pair only once.

  The deterministic construction starts with the parse tree for the regular expression, observing that each leaf represents an alphabet symbol in the pattern. After recognizing a prefix of the text, we can be left in some subset of these possible positions, which would correspond to a state in the finite automaton. The *derivatives* method builds up this automaton state by state as it is needed. Even so, some regular expressions of length m require $O(2^m)$ states in any DFA implementing them, such as $(a+b)^*a(a+b)(a+b)\ldots(a+b)$. There is no way to avoid this exponential space blowup. Fortunately it takes linear time to simulate an input string on any DFA, regardless of the size of the automaton.

Implementations: *Grail+* is a C++ package for symbolic computation with finite automata and regular expressions. Grail enables one to convert between different machine representations and to minimize automata. It can handle large machines defined on large alphabets. All code and documentation are accessible from *http://www.csd.uwo.ca/Research/grail*, as well as pointers to a variety of other automaton packages. Commercial use of Grail is not allowed without approval, although it is freely available to students and educators.

The AT&T Finite State Machine Library (FSM) is a set of general-purpose UNIX software tools for building, combining, optimizing, and searching weighted finite-state acceptors and transducers. It supports automata with more than ten million states and transitions. See *http://www.research.att.com/~fsmtools/fsm/*.

JFLAP (Java Formal Languages and Automata Package) is a package of graphical tools for learning the basic concepts of automata theory. Included are functions to convert between DFAs, NFAs, and regular expressions, and minimize the resulting automata. High-level automata are also supported, including context-free languages and Turing machines. *JFLAP* is available at *http://www.jflap.org/*. A related book [RF06] is also available.

FIRE Engine provides production-quality implementations of finite automata and regular expression algorithms. Several finite automaton

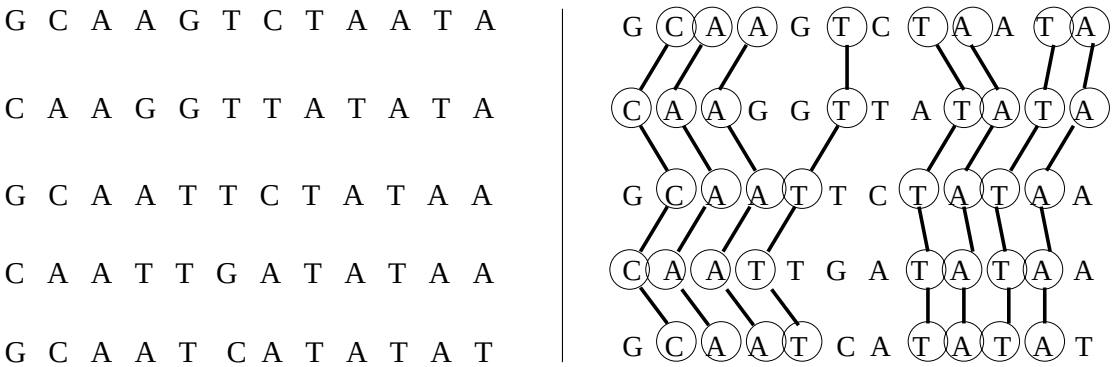
minimization algorithms have been implemented, including Hopcroft's $O(n \lg n)$ algorithm. Both deterministic and nondeterministic automata are supported. It is available at *http://www.fastar.org/* and, with certain enhancements, at *www.eti.pg.gda.pl/∼jandac/minim.html*.

Notes: Aho [Aho90] provides a good survey on algorithms for pattern matching, with a particularly clear exposition for the case where the patterns are regular expressions. The technique for regular expression pattern matching with ϵ-moves is due to Thompson [Tho68]. Other expositions on finite automaton pattern matching include [AHU74]. Expositions on finite automata and the theory of computation include [HMU06, Sip05]

The major annual meeting of interest in this field is the *Conference on Implementations and Applications of Automata* (CIAA). Pointers to current and previous meetings with associated software are available at *http://tln.li.univ-tours.fr/ciaa/*.

Hopcroft [Hop71] gave an optimal $O(n \lg n)$ algorithm for minimizing the number of states in DFAs. The derivatives method of constructing a finite state machine from a regular expression is due to Brzozowski [Brz64] and has been expanded upon in [BS86]. Expositions on the derivatives method includes Conway [Con71]. Recent work on incremental construction and optimization of automata includes [Wat03]. The problems of compressing a DFA to a minimum NFA [JR93] and testing the equivalence of two nondeterministic finite state machines [SM73] are both PSPACE-complete.

Related Problems: Satisfiability (see page 472). string matching (see page 628).



INPUT OUTPUT

18.8 Longest Common Substring/Subsequence

Input description: A set S of strings $S_1, \ldots, S_n$.

Problem description: What is the longest string S' such that all the characters of S' appear as a substring or subsequence of each S_i, $1 \leq i \leq n$?

Discussion: The problem of longest common substring/subsequence arises whenever we search for similarities across multiple texts. A particularly important application is finding a consensus among biological sequences. The genes for building proteins evolve with time, but the functional regions must remain consistent in order for them to work correctly. The longest common subsequence of the same gene in different species provides insight into what has been conserved over time.

The longest common subsequence problem for two strings is a special case of edit distance (see Section 18.4 (page 631)), when substitutions are forbidden and exact character match, insert, and delete are the only allowable edit operations. Under these conditions, the edit distance between P and T is $n + m - 2|lcs(P, T)|$, since we can delete the missing characters from P to the $lcs(P, T)$ and insert the missing characters from T to transform P to T.

Issues arising include

- *Are you looking for a common substring?* – In detecting plagiarism, we might need to find the longest phrase shared between two or more documents. Since phrases are strings of consecutive characters, here we need the longest common *substring* between the texts.

  The longest common substring of a set of strings can be identified in linear time using suffix trees, as discussed in Section 12.3 (page 377). The trick is to build a suffix tree containing all the strings, label each leaf with the input

string it represents, and then do a depth-first traversal to identify the deepest node with descendants from each input string.

- *Are you looking for a common scattered subsequence?* – For the rest of our discussion here, we restrict attention to finding common scattered subsequences. This algorithm is a special case of the dynamic program edit-distance computation. Indeed, an implementation in C is given on page 288.

  Let $M[i,j]$ denote the number of characters in the longest common substring of $S[1],\ldots,S[i]$ and $T[1],\ldots,T[j]$. When $S[i] \neq T[j]$, there is no way the last pair of characters could match, so $M[i,j] = \max(M[i,j-1], M[i-1,j])$. But if $S[i] = T[j]$, we have the option to select this character for our substring, so $M[i,j] = \max(M[i-1,j-1]+1, M[i-1,j], M[i,j-1])$.

  This recurrence computes the length of the longest common subsequence in $O(nm)$ time. We can reconstruct the actual common substring by walking backward from $M[n,m]$ and establishing which characters were matched along the way.

- *What if there are relatively few sets of matching characters?* – There is a faster algorithm for strings that do not contain too many copies of the same character. Let r be the number of pairs of positions (i,j) such that $S_i = T_j$. Thus, r can be as large as mn if both strings consist entirely of the same character, but $r = n$ if both strings are permutations of $\{1,\ldots,n\}$. This technique treats the pairs of r as defining points in the plane.

  The complete set of r such points can be found in $O(n+m+r)$ time using bucketing techniques. We create a bucket for each alphabet symbol c and each string (S or T), then partition the positions of each character of the string into the appropriate bucket. We then create a point (s,t) from every pair $s \in S_c$ and $t \in T_c$ in the buckets S_c and T_c.

  A common subsequence describes a monotonically nondecreasing path through these points, meaning the path only moves up and to the right. The longest such path can be found in $O((n+r)\lg n)$ time. We sort the points in order of increasing x-coordinate, breaking ties in favor of increasing y-coordinate. We insert points one by one in this order, and maintain the minimum terminal y-coordinate of any path going through exactly k points for each k, for $1 \leq k \leq n$. The new point (p_x, p_y) changes exactly one of these paths, either identifying a new longest subsequence or reducing the y-coordinate of the shortest path whose endpoint lies above p_y.

- *What if the strings are permutations?* – Permutations are strings without repeating characters. Two permutations define n pairs of matching characters, and so the above algorithm runs in $O(n \lg n)$ time. A particularly important case occurs in finding the longest *increasing* subsequence of a numerical sequence. Sorting the sequence and then replacing each number by

its rank defines a permutation p. The longest common subsequence of p and $\{1, 2, 3, \ldots, n\}$ gives the longest increasing subsequence.

- *What if we have more than two strings to align?* – The basic dynamic programming algorithm can be generalized to k strings, taking $O(2^k n^k)$ time, where n is the length of the longest string. This algorithm is exponential in the number of strings k, and so it will likely be too expensive for more than a few strings. Furthermore, the problem is NP-complete, so no better exact algorithm is destined to come along soon.

  Many heuristics have been proposed for multiple sequence alignment. They often start by computing the pairwise alignment for each of the $\binom{k}{2}$ pairs of strings. One approach then replaces the two most similar sequences with a single merged sequence, and repeats until all these alignments have been merged into one. The catch is that two strings often have many different alignments of optimal cost. The "right" alignment to pick depends upon the remaining sequences to merge, and is hence unknowable to the heuristic.

Implementations: Several programs are available for multiple sequence alignment of DNA/protein sequence data. *ClustalW* [THG94] is a popular and well-regarded program for multiple alignment of protein sequences. It is available at *http://www.ebi.ac.uk/Tools/clustalw/*. Another respectable option is the *MSA* package for multiple sequence alignment [GKS95], which is available at *http://www.ncbi.nlm.nih.gov/CBBresearch/Schaffer/msa.html*.

Any of the dynamic programming-based approximate string matching programs of Section 18.4 (page 631) can be used to find the longest common subsequence of two strings. More specialized implementations in Perl, Java, and C are available at *http://www.bioalgorithms.info/downloads/code/*.

Combinatorica [PS03] provides a Mathematica implementation of an algorithm to construct the longest increasing subsequence of a permutation, which is a special case of longest common subsequence. This algorithm is based on Young tableaux rather than dynamic programming. See Section 19.1.9 (page 661).

Notes: Surveys of algorithmic results on longest common subsequence (LCS) problems include [BHR00, GBY91]. The algorithm for the case where all the characters in each sequence are distinct or infrequent is due to Hunt and Szymanski [HS77]. Expositions of this algorithm include [Aho90, Man89]. There has been a surprising amount of recent work on this problem, including efficient bit-parallel algorithms for LCS [CIPR01]. Masek and Paterson [MP80] solve longest common subsequence in $O(mn/\log(\min\{m, n\}))$ for constant-sized alphabets, using the four Russians technique.

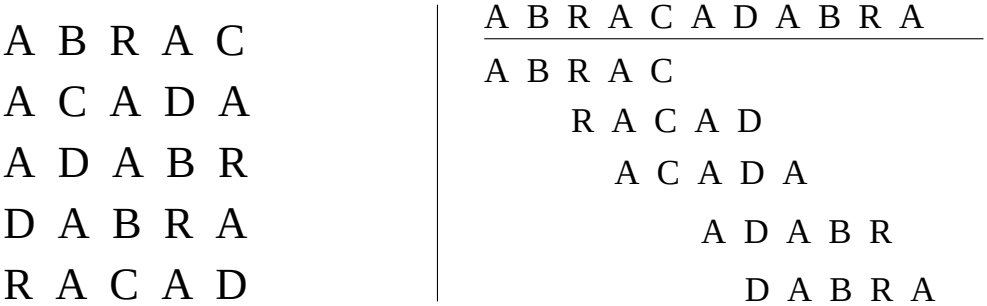
Construct two random n-character strings on an alphabet of size α. What is the expected length of their LCS? This problem has been extensively studied, with an excellent survey by Dancik [Dan94].

Multiple sequence alignment for computational biology is large field, with the books of Gusfield [Gus97] and Durbin [DEKM98] serving as excellent introductions. See [Not02]

for a more recent survey. The hardness of multiple sequence alignment follows from that of shortest common subsequence for large sets of strings [Mai78].

We motivated the problem of longest common substring with the application of plagiarism detection. See [SWA03] for the interesting details of how to implement a plagiarism detector for computer programs.

Related Problems: Approximate string matching (see page 631), shortest common superstring (see page 654).



INPUT OUTPUT

18.9 Shortest Common Superstring

Input description: A set of strings $S = \{S_1, \ldots, S_m\}$.

Problem description: Find the shortest string S' that contains each string S_i as a substring of S'.

Discussion: Shortest common superstring arises in a variety of applications. A casino gambling addict once asked me how to reconstruct the pattern of symbols on the wheels of a slot machine. On every spin, each wheel turns to a random position, displaying the selected symbol as well as the symbols immediately before/after it. Given enough observations of the slot machine, the symbol order for each wheel can be determined as the shortest common (circular) superstring of the observed symbol triples.

Another application of shortest common superstring is data/matrix compression. Suppose we are given a sparse $n \times m$ matrix M, meaning that most elements are zero. We can partition each row into m/k runs of k elements, and construct the shortest common superstring S' of all these runs. We can now represent the matrix by this superstring plus an $n \times m/k$ array of pointers denoting where each of these runs starts in S'. Any particular element $M[i, j]$ can still be accessed in constant time, but there will be substantial space savings when $|S| << mn$.

Perhaps the most compelling application is in DNA sequence assembly. Machines readily sequence fragments of about 500 base pairs or characters of DNA, but the real interest is in sequencing large molecules. Large-scale "shotgun" sequencing clones many copies of the target molecule, breaks them randomly into fragments, sequences the fragments, and then proposes the shortest superstring of the fragments as the correct sequence.

Finding a superstring of a set of strings is not difficult, since we can simply concatenate them together. Finding the *shortest* such string is what's problematic.

Indeed, shortest common superstring is NP-complete for all reasonable classes of strings.

Finding the shortest common superstring can easily be reduced to the traveling salesman problem (see Section 16.4 (page 533)). Create an overlap graph G where vertex v_i represents string S_i. Assign edge (v_i, v_j) weight equal to the length of S_i minus the overlap of S_j with S_i. Thus, $w(v_i, v_j) = 1$ for $S_i = abc$ and $S_j = bcd$. The minimum weight path visiting all the vertices defines the shortest common superstring. These edge weights are not symmetric; note that $w(v_j, v_i) = 3$ for the example above. Unfortunately, asymmetric TSP problems are much harder to solve in practice than symmetric instances.

The greedy heuristic provides the standard approach to approximating shortest common superstring. Identify which pair of strings have the maximum overlap. Replace them by the merged string, and repeat until only one string remains. This heuristic can actually be implemented in linear time. The seemingly most time-consuming part is in building the overlap graph. The brute-force approach to finding the maximum overlap of two length-l strings takes $O(l^2)$ for each of $O(n^2)$ string pairs. However, faster times are possible by using suffix trees (see Section 12.3 (page 377)). Build a tree containing all suffixes of all strings of S. String S_i overlaps with S_j iff a suffix of S_i matches the prefix of S_j—an event defined by a vertex of the suffix tree. Traversing these vertices in order of distance from the root defines the appropriate merging order.

How well does the greedy heuristic perform? It can certainly be fooled into creating a superstring that is twice as long as optimal. The optimal merging order for strings $c(ab)^k$, $(ba)^k$, and $(ab)^k c$ is left to right. But greedy starts by merging the first and third string, leaving the middle one no overlap possibility. The greedy superstring can never be worse than 3.5 times optimal, and usually will be a lot better in practice.

Building superstrings becomes more difficult when given both positive and negative strings, where each of the negative strings are forbidden to be a substring of the final result. The problem of deciding whether *any* such consistent substring exists is NP-complete, unless you are allowed to add an extra character to the alphabet to use as a spacer.

Implementations: Several high-performance programs for DNA sequence assembly are available. Such programs correct for sequencing errors, so the final result is not necessarily a superstring of the input reads. At the very least, they will serve as excellent models if you really need a short proper superstring.

CAP3 (Contig Assembly Program) [HM99] and *PCAP* [HWA+03] are the latest in a series of assemblers by Xiaoqiu Huang and his collaborators, which are available from *http://seq.cs.iastate.edu/*. They have been used on mammalian scale assembly projects involving hundreds of millions of bases.

The Celera assembler that originally sequenced the human genome is now available as open source. See *http://sourceforge.net/projects/wgs-assembler/*.

Notes: The shortest common superstring (SCS) problem and its application to DNA shotgun assembly are ably surveyed in [MKT07, Mye99a]. Kececioglu and Myers [KM95] report on an algorithm for this more general version of shortest common superstring, where the strings are assumed to have character substitution errors. Their paper is recommended reading to anyone interested in fragment assembly.

Blum et al. [BJL+94] gave the first constant-factor approximation algorithms for shortest common superstring, using a variation of the greedy heuristic. More recent research has beaten this constant down to 2.5 [Swe99], progress towards the expected factor-two result. The best approximation ratio so far proven for the standard greedy heuristic is 3.5 [KS05a]. Fast implementations of such heuristics are described in [Gus94].

Experiments on shortest common superstring heuristics are reported in [RBT04], which suggest that greedy heuristics typically produce solutions within 1.4% of optimal for a reasonable class of inputs. Experiments with genetic algorithm approaches are reported in [ZS04]. Analytical results [YZ99] demonstrate very little compression on the SCS of random sequences largely because the expected overlap length of any two random strings is small.

Related Problems: Suffix trees (see page 377), text compression (see page 637).

19

Algorithmic Resources

This chapter briefly describes resources that the practical algorithm designer should be familiar with. Although some of this information has appeared elsewhere in the catalog, the most important pointers are collected here for general reference.

19.1 Software Systems

In this section, we describe several particularly comprehensive implementations of combinatorial algorithms, all of which are downloadable over the Internet. Although these codes are mentioned in the relevant sections of the catalog, they are substantial enough to warrant further attention.

A good algorithm designer does not reinvent the wheel, and a good programmer does not rewrite code that other people have written. Picasso put it best: "Good artists borrow. Great artists steal."

However, here is a word of caution about stealing. Many of the codes described in this book have been made available for research or educational use only. Commercial use may require a licensing arrangement with the author. I urge you to respect this. Licensing terms from academic institutions are usually quite modest. The recognition that industry is using a particular code is important to the authors, often more important than the money involved. This can lead to enhanced support or future releases of the software. Do the right thing and get a license. Information about terms or whom to contact is usually available embedded within the documentation, or available at the source's website.

Although many of the systems we describe here may be available by accessing our algorithm repository, *http://www.cs.sunysb.edu/∼algorith* we encourage you to get them from the original sites instead of Stony Brook. There are three reasons. First, the version on the original site is *much* more likely to be up-to-date. Second,

S.S. Skiena, *The Algorithm Design Manual*, 2nd ed., DOI: 10.1007/978-1-84800-070-4_19,
© Springer-Verlag London Limited 2008

there are often supporting files and documentation that we did not download that may be of interest to you. Finally, many authors monitor the downloads of their codes, and so you deny them a well-earned thrill if you don't take them from the homepage.

19.1.1 LEDA

LEDA, for *Library of Efficient Data types and Algorithms*, is perhaps the best single resource available to support combinatorial computing. *LEDA* was originally developed by a group at Max-Planck-Instutut in Saarbrücken, Germany, including Kurt Mehlhorn, Stefan Näher, Stefan Schirra, Christian Uhrig, and Christoph Burnikel. *LEDA* is unique because of (1) the algorithmic sophistication of its developers, and (2) the level of continuity and resources invested in the project.

What *LEDA* offers is a complete collection of well-implemented C++ data structures and types. Particularly useful is the graph type, which supports all the basic operations one needs in an intelligent way, although this generality comes at some cost in size and speed over handcrafted implementations. A useful library of graph algorithms is included, which illustrates how cleanly and concisely these algorithms can be implemented using the LEDA data types. Good implementations of the most important data structures supporting such common data types as dictionaries and priority queues are provided. There are also algorithms and data structures for computational geometry, including support for visualization. For more, see the book [MN99].

Since 2001, *LEDA* has been exclusively available from Algorithmic Solutions Software GmbH (*http://www.algorithmic-solutions.com/*). This ensures professional-quality support, and new releases appear often. The great news is that a free edition containing all the basic data structures (including dictionaries, priority queues, graphs, and numerical types) was released February 2008. No source code or advanced algorithms are provided with the free edition. However, the licencing fees for the full library are not outlandish and free trial downloads are available.

19.1.2 CGAL

The *Computational Geometry Algorithms Library* or *CGAL* provides efficient and reliable geometric algorithms in C++. It is extremely comprehensive, offering a rich variety of triangulations, Voronoi diagrams, operations on polygons and polyhedra, line/curve arrangements, alpha-shapes, convex-hull algorithms, geometric search structures, and more. Many work in three dimensions and some beyond.

CGAL (*www.cgal.org*) should be the first place to go for serious geometric computing, although you should expect to spend some start-up time getting oriented to the *CGAL* way of thinking. *CGAL* is distributed under a dual-license scheme. It can be used together with open source software free of charge but using *CGAL* in other contexts requires obtaining a commercial license.

19.1.3 Boost Graph Library

Boost (*www.boost.org*) provides a well-regarded collection of free peer-reviewed portable C++ source libraries. The Boost license encourages both commercial and noncommercial use.

The Boost Graph Library [SLL02] (*http://www.boost.org/libs/graph/doc*) is perhaps most relevant for the readers of this book. Implementations of adjacency lists, matrices, and edge lists are included, along with a reasonable library of basic graph algorithms. Its interface and components are generic in the same sense as the C++ Standard Template Library (STL). Other Boost libraries of interest include those for string/text processing and math/numeric computation.

19.1.4 GOBLIN

The *Graph Object Library for Network Programming Problems* (GOBLIN) is a C++ class library that broadly focuses on graph optimization problems. These include several varieties of shortest path, minimum spanning tree, and connected component algorithms, plus particularly strong coverage of network flows and matching. Finally, a generic branch-and-bound module is used to solve such hard problems as independent set and vertex coloring.

GOBLIN was written and is maintained by Christian Fremuth-Paeger at the University of Augsberg. It is available under GNU lesser public licence from *http://www.math.uni-augsburg.de/~fremuth/goblin.html*. A spiffy Tcl/Tk interface is provided. GOBLIN is presumably not as robust as *Boost* or *LEDA*, but contains several algorithms not present in either of them.

19.1.5 Netlib

Netlib (*www.netlib.org*) is an online repository of mathematical software that contains a large number of interesting codes, tables, and papers. Netlib is a compilation of resources from a variety of places, with fairly detailed indices and search mechanisms. Netlib is important because of its breadth and ease of access. Whenever you need a specialized piece of mathematical software, you should look here first.

The Guide to Available Mathematical Software (GAMS), is an indexing service for Netlib and other related software repositories that can help you find what you want. Check it out at *http://gams.nist.gov*. GAMS is a service of the National Institute of Standards and Technology (NIST).

19.1.6 Collected Algorithms of the ACM

An early mechanism for the distribution of useful algorithm implementations was the *Collected Algorithms of the ACM* (*CALGO*). It first appeared in *Communications of the ACM* in 1960, covering such famous algorithms as Floyd's linear-time build heap algorithm. More recently, it has been the province of the *ACM Transactions on Mathematical Software*. Each algorithm/implementation is described

in a brief journal article, with the implementation validated and collected. These implementations are maintained at *http://www.acm.org/calgo/* and at Netlib.

Over 850 algorithms have appeared to date. Most of the codes are in Fortran and are relevant to numerical computing, although several interesting combinatorial algorithms have slithered their way into CALGO. Since the implementations have been refereed, they are presumably more reliable than most comparable software.

19.1.7 SourceForge and CPAN

SourceForge (*http://sourceforge.net/*) is the largest open source software development website, with over 160,000 registered projects. Most are of highly limited interest, but there is a lot of good stuff to be found. These include graph libraries such as *JUNG* and *JGraphT*, optimization engines such as *lpsolve* and *JGAP*, and much more.

CPAN (*http://www.cpan.org/*) is the Comprehensive Perl Archive Network. This enormous collection of Perl modules and scripts is where you should look before trying to implement anything in Perl.

19.1.8 The Stanford GraphBase

The Stanford GraphBase is an interesting program for several reasons. First, it was composed as a "literate program," meaning that it was written to be read. If anybody's programs deserve to be read, it is Knuth's, and [Knu94] contains the full source code of the system. The programming language/environment is CWEB, which permits the mixing of text and code in particularly expressive ways.

The GraphBase contains implementations of several important combinatorial algorithms, including matching, minimum spanning trees, and Voronoi diagrams, as well as specialized topics like constructing expander graphs and generating combinatorial objects. Finally, it contains programs for several recreational problems, including constructing word ladders (flour-floor-flood-blood-brood-broad-bread) and establishing dominance relations among football teams. Check it out at *http://www-cs-faculty.stanford.edu/~knuth/sgb.html*.

Although the GraphBase is fun to play with, it is not really suited for building general applications on top of. The GraphBase is perhaps most useful as an instance generator for constructing a wide variety of graphs to serve as test data. It incorporates graphs derived from interactions of characters in famous novels, Roget's thesaurus, the Mona Lisa, and the economy of the United States. Furthermore, because of its machine-independent random number generators, the GraphBase provides a way to construct random graphs that can be reconstructed elsewhere, making them perfect for experimental comparisons of algorithms.

19.1.9 Combinatorica

Combinatorica [PS03] is a collection of over 450 algorithms for combinatorics and graph theory written in Mathematica. These routines have been designed to work together, enabling one to readily experiment with discrete structures. *Combinatorica* has been widely used for both research and education.

Although (in my totally unbiased opinion) *Combinatorica* is more comprehensive and better integrated than other libraries of combinatorial algorithms, it is also the slowest such system available. Credit for all of these properties is largely due to Mathematica, which provides a very high-level, functional, interpreted, and thus inefficient programming language. *Combinatorica* is best for finding quick solutions to small problems, and (if you can read Mathematica code) as a terse exposition of algorithms for translation into other languages.

Check out *http://www.combinatorica.com* for the latest release and associated resources. It is also included with the standard Mathematica distribution in the directory *Packages/DiscreteMath/Combinatorica.m*.

19.1.10 Programs from Books

Several books on algorithms include working implementations of the algorithms in a real programming language. Although these implementations are intended primarily for exposition, they can also be useful for computation. Since they are typically small and clean, they can prove the right foundation for simple applications.

The most useful codes of this genre are described below. Most are available from the algorithm repository, *http://www.cs.sunysb.edu/∼algorith*.

Programming Challenges

If you like the C code that appeared in the first half of the text, you should check out the programs I wrote for my book *Programming Challenges* [SR03]. Perhaps most useful are additional examples of dynamic programming, computational geometry routines like convex hull, and a bignum integer arithmetic package. This algorithm library is available at *http://www.cs.sunysb.edu/∼skiena/392/programs/* or at *http://www.programming-challenges.com*.

Combinatorial Algorithms for Computers and Calculators

Nijenhuis and Wilf [NW78] specializes in algorithms for constructing basic combinatorial objects such as permutations, subsets, and partitions. Such algorithms are often very short, but they are hard to locate and usually surprisingly subtle. Fortran routines for all of the algorithms are provided, as well as a discussion of the theory behind each of them. The programs are usually short enough that it is reasonable to translate them directly into a more modern programming language, as I did in writing *Combinatorica* (see Section 19.1.9). Both random and sequential

generation algorithms are provided. Descriptions of more recent algorithms for several problems, without code, are provided in [Wil89].

These programs are now available from our algorithm repository website. We tracked them down from Neil Sloane, who had them on a magnetic tape, while the original authors did not! In [NW78], Nijenhuis and Wilf set the proper standard of statistically testing the output distribution of each of the random generators to establish that they really appear uniform. We encourage you to do the same before using these programs to verify that nothing has been lost in transit.

Computational Geometry in C

O'Rourke [O'R01] is perhaps the best practical introduction to computational geometry, because of its careful and correct C language implementations of all the main algorithms of computational geometry. Fundamental geometric primitives, convex hulls, triangulations, Voronoi diagrams, and motion planning are all included. Although they were implemented primarily for exposition rather than production use, they should be quite reliable. The codes are available from *http://maven.smith.edu/∼orourke/code.html*.

Algorithms in C++

Sedgewick's popular algorithms text [Sed98, SS02] comes in several different language editions, including C, C++, and Java. This book distinguishes itself through its use of algorithm animation and in its broad topic coverage, including numerical, string, and geometric algorithms.

The language-specific parts of the text consist of many small code fragments, instead of full programs or subroutines. They are best thought of as models, instead of working implementations. Still, the program fragments from the C++ edition have been made available from *http://www.cs.princeton.edu/∼rs/*.

Discrete Optimization Algorithms in Pascal

This is a collection of 28 programs for solving discrete optimization problems, appearing in the book by Syslo, Deo, and Kowalik [SDK83]. The package includes programs for integer and linear programming, the knapsack and set cover problems, traveling salesman, vertex coloring, and scheduling, as well as standard network optimization problems. They have been made available from the algorithm repository at *http://www.cs.sunysb.edu/∼algorith*.

This package is noteworthy for the operations-research flavor of the problems and algorithms selected. The algorithms have been selected to solve problems, rather than purely expository purposes.

19.2 Data Sources

It is often important to have interesting data to feed your algorithms, to serve as test data to ensure correctness or to compare different algorithms for raw speed. Finding good test data can be surprisingly difficult. Here are some pointers:

- *TSPLIB* – This well-respected library of test instances for the traveling salesman problem [Rei91] provides the standard collection of hard instances of TSPs. TSPLIB instances are large, real-world graphs, derived from applications such as circuit boards and networks. TSPLIB is available from *http://www.iwr.uni-heidelberg.de/groups/comopt/software/TSPLIB95/* Somewhat older instances are also available from Netlib.
- *Stanford GraphBase* – Discussed in Section 19.1.8, this suite of programs by Knuth provides portable generators for a wide variety of graphs. These include graphs arising from distance matrices, arts, and literature, as well as graphs of more theoretical interest.
- *DIMACS Challenge data* – A series of DIMACS Challenge workshops have focused on evaluating algorithm implementations of graph, logic, and data structure problems. Instance generators for each problem have been developed, with the focus on constructing difficult or representative test data. The products of the DIMACS Challenges are all available from *http://dimacs.rutgers.edu/Challenges*.

19.3 Online Bibliographic Resources

The Internet has proven to be a fantastic resource for people interested in algorithms, as it has for many other subjects. What follows is a highly selective list of the resources that I use most often. All should be in the tool chest of every algorist.

- *ACM Digital Library* – This collection of bibliographic references provides links to essentially every technical paper ever published in computer science. Check out what is available at *http://portal.acm.org/*.
- *Google Scholar* – This free resource (*http://scholar.google.com/*) restricts Web searches to things that look like academic papers, often making it a sounder search for serious information than a general Web search. Particularly useful is the ability to see which papers cite a given paper. This lets you update an old reference to see what has happened since publication, and helps to judge the significance of a particular article.
- *Amazon.com* – This comprehensive catalog of books (*www.amazon.com*) is surprisingly useful for finding relevant literature for algorithmic problems, particularly since many recent books have been digitized and placed in it's index.

19.4 Professional Consulting Services

Algorist Technologies (*http://www.algorist.com*) is a consulting firm that provides its clients with short-term, expert help in algorithm design and implementation. Typically, an Algorist consultant is called in for one to three days worth of intensive, onsite discussion and analysis with the client's own development staff. Algorist has built an impressive record of performance improvements with several companies and applications. We provide longer-term consulting and contracting services as well.

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Index