

CHAPTER Fundamentals of algorithms

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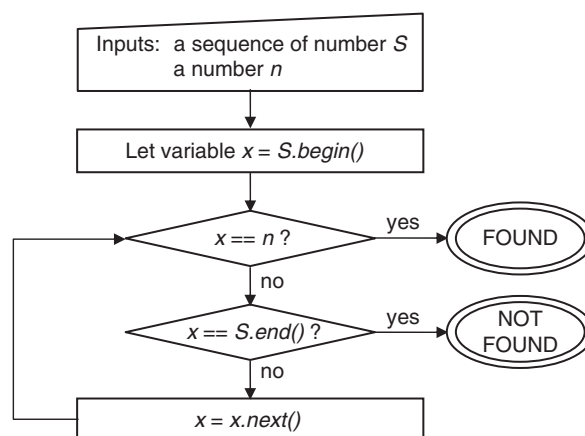
ABOUT THIS CHAPTER

In this chapter, we will go through the fundamentals of algorithms that are essential for the readers to appreciate the beauty of various EDA technologies covered in the rest of the book. For example, many of the EDA problems can be either represented in graph data structures or transformed into graph problems. We will go through the most representative ones in which the efficient algorithms have been well studied.

The readers should be able to use these graph algorithms in solving many of their research problems. Nevertheless, there are still a lot of the EDA problems that are naturally difficult to solve. That is to say, it is computationally infeasible to seek for the optimal solutions for these kinds of problems. Therefore, heuristic algorithms that yield suboptimal, yet reasonably good, results are usually adopted as practical approaches. We will also cover several selected heuristic algorithms in this chapter. At the end, we will talk about the mathematical programming algorithms, which provide the theoretical analysis for the problem optimality. We will especially focus on the mathematical programming problems that are most common in the EDA applications.

4.1 INTRODUCTION

An algorithm is a sequence of well-defined instructions for completing a task or solving a problem. It can be described in a natural language, pseudocode, a flow-chart, or even a programming language. For example, suppose we are interested in knowing whether a specific number is contained in a given sequence of numbers. By traversing the entire number sequence from a certain beginning number

**FIGURE 4.1**

Flowchart of the “Linear Search” algorithm.

to a certain ending number, we use a search algorithm to find this specific number. Figure 4.1 illustrates this intuitive algorithm known as *linear search*.

Such kinds of algorithms can be implemented in a computer program and then used in real-life applications [Knuth 1968; Horowitz 1978]. However, the questions that must be asked before implementation are: “Is the algorithm efficient?” “Can the algorithm complete the task within an acceptable amount of time for a specific set of data derived from a practical application?” As we will see in the next section, there are methods for quantifying the efficiency of an algorithm. For a given problem, different algorithms can be applied, and each of them has a different degree of efficiency. Such metrics for measuring an algorithm’s efficiency can help answer the preceding questions and aid in the selection of the best possible algorithm for the task.

Devising an efficient algorithm for a given EDA problem could be challenging. Because a rich collection of efficient algorithms already exists for a set of standard problems where data are represented in the form of graphs, one possible approach is to model the given problem as a graph problem and then apply a known, efficient algorithm to solve the modeled graph problem. In Section 4.3, we introduce several graph algorithms that are commonly used for a wide range of EDA problems.

Many EDA problems are intrinsically difficult, because finding an optimal solution within a reasonable runtime is not always possible. For such problems, certain *heuristic algorithms* can be applied to find an acceptable solution first. If time or computer resources permit, such algorithms can further improve the result incrementally.

In addition to modeling EDA problems in graphs, it is sometimes possible to transform them into certain mathematical models, such as linear inequalities or nonlinear equations. The primary advantage of modeling an EDA problem with

a mathematical formula is that there are many powerful tools that can automatically handle these sorts of mathematical problems. They may yield better results than the customized heuristic algorithms. We will briefly introduce some of these useful mathematical programming techniques near the end of this chapter.

4.2 COMPUTATIONAL COMPLEXITY

A major criterion for a good algorithm is its **efficiency**—that is, how much **time** and **memory** are required to solve a particular problem. Intuitively, time and memory can be measured in real units such as seconds and megabytes. However, these measurements are not subjective for comparisons between algorithms, because they depend on the computing power of the specific machine and on the specific data set. To standardize the measurement of algorithm efficiency, the **computational complexity theory** was developed [Ullman 1984; Papadimitriou 1993, 1998; Wilf 2002]. This allows an algorithm's efficiency to be estimated and expressed conceptually as a mathematical function of its *input size*.

Generally speaking, the *input size* of an algorithm refers to the number of items in the input data set. For example, when sorting n words, the input size is n . Notice that the conventional symbol for input size is n . It is also possible for an algorithm to have an input size with multiple parameters. Graph algorithms, which will be introduced in Section 4.3, often have input sizes with two parameters: the number of vertices $|V|$ and the number of edges $|E|$ in the graph.

Computational complexity can be further divided into **time complexity** and **space complexity**, which estimate the time and memory requirements of an algorithm, respectively. In general, time complexity is considered much more important than space complexity, in part because the memory requirement of most algorithms is lower than the capacity of current machines. In the rest of the section, all calculations and comparisons of algorithm efficiency refer to time complexity as **complexity** unless otherwise specified. Also, time complexity and running time can be used interchangeably in most cases.

The time complexity of an algorithm is calculated on the basis of the number of required elementary computational steps that are interpreted as a function of the input size. Most of the time, because of the presence of conditional constructs (e.g., if-else statements) in an algorithm, the number of necessary steps differs from input to input. Thus, *average-case complexity* should be a more meaningful characterization of the algorithm. However, its calculations are often difficult and complicated, which necessitates the use of a *worst-case complexity* metric. An algorithm's worst-case complexity is its complexity with respect to the worst possible inputs, which gives an upper bound on the average-case complexity. As we shall see, the worst-case complexity may sometimes provide a decent approximation of the average-case complexity.

The calculation of computational complexity is illustrated with two simple examples in Algorithm 4.1 and 4.2. Each of these entails the process of looking

up a word in a dictionary. The input size n refers to the total number of words in the dictionary, because every word is a possible target. The first algorithm—linear search—is presented in Algorithm 4.1. It starts looking for the target word t from the first word in the dictionary ($Dic[0]$) to the last word ($Dic[n-1]$). The conclusion “not found” is made only after every word is checked. On the other hand, the second algorithm—binary search—takes advantage of the alphabetic ordering of the words in a dictionary. It first compares the word in the middle of the dictionary ($Dic[mid]$) with the target t . If t is alphabetically “smaller” than $Dic[mid]$, t must rest in the front part of the dictionary, and the algorithm will then focus on the front part of the word list in the next iteration (line 5 of `Binary_Search`), and *vice versa*. In every iteration, the middle of the search region is compared with the target, and one half of the current region will be discarded in the next iteration. Binary search continues until the target word t is matched or not found at all.

Algorithm 4.1 Linear Search Algorithm

`Linear_Search(Array_of_words Dic[n], Target t)`

1. **for** counter ctr from 0 to $n-1$
 2. **if** ($Dic[ctr]$ is t) **return** $Dic[ctr]$;
 3. **return** NOT_FOUND;
-

Algorithm 4.2 Binary Search Algorithms

`Binary_Search(Array_of_words Dic[n], Target t)`

1. Position $low = 0$, $high = n-1$;
 2. **while** ($low \leq high$) **do**
 3. Position $mid = (low + high)/2$;
 4. **if** ($Dic[mid] < t$) $low = mid$;
 5. **else if** ($Dic[mid] > t$) $high = mid$;
 6. **else** // $Dic[mid]$ is t
 7. **return** $Dic[mid]$;
 8. **end if**
 9. **end while**
 10. **return** NOT_FOUND;
-

In linear search, the worst-case complexity is obviously n , because every word must be checked if the dictionary does not contain the target word at all. Different target words require different numbers of executions of lines 1–2 in `Linear_Search`, yet on average, $n/2$ times of checks are required.

Thus, the average-case complexity is roughly $n/2$. Binary search is apparently quicker than linear search. Because in every iteration of the *while* loop in `Binary_Search` one-half of the current search area is discarded, at most $\log_2 n$ (simplified as $\lg n$ in the computer science community) of lookups are required—the worst-case complexity. n is clearly larger than $\lg n$, which proves that binary search is a more efficient algorithm. Its average-case complexity can be calculated as in Equation (4.1) by adding up all the possible numbers of executions and dividing the result by n .

$$\begin{aligned} \text{average-case-complexity} &= \left(1 \cdot 1 + 2 \cdot 2 + 4 \cdot 3 + 8 \cdot 4 + \dots + \frac{n}{2} \cdot \lg n \right) / n \\ &= \lg n - 1 + \frac{3}{n} \end{aligned} \quad (4.1)$$

4.2.1 Asymptotic notations

In computational complexity theory, not all parts of an algorithm's running time are essential. In fact, only the **rate of growth** or the **order of growth** of the running time is typically of most concern in comparing the complexities of different algorithms. For example, consider two algorithms A and B, where A has longer running time for smaller input sizes, and B has a higher rate of growth of running time as the input size increases. Obviously, the running time of B will outnumber that of A for input sizes greater than a certain number. As in real applications, the input size of a problem is typically very large, algorithm B will always run more slowly, and thus we will consider it as the one with higher computational complexity.

Similarly, it is also sufficient to describe the complexity of an algorithm considering only the factor that has highest rate of growth of running time. That is, if the computational complexity of an algorithm is formulated as an equation, we can then focus only on its dominating term, because other lower-order terms are relatively insignificant for a large n . For example, the average-case complexity of `Binary_Search`, which was shown in Equation (4.1), can be simplified to only $\lg n$, leaving out the terms -1 and $3/n$. Furthermore, we can also ignore the dominating term's constant coefficient, because it contributes little information for evaluating an algorithm's efficiency. In the example of `Linear_Search` in Algorithm 4.1, its worst-case complexity and average-case complexity— n and $n/2$, respectively—are virtually equal under this criterion. In other words, they are said to have asymptotically equal complexity for larger n and are usually represented with the following *asymptotic notations*.

Asymptotic notations are symbols used in computational complexity theory to express the efficiency of algorithms with a focus on their orders of growth. The three most used notations are O -notation, Ω -notation, and Θ -notation.

| | Also called | $n = 100$ | $n = 10,000$ | $n = 1,000,000$ |
|--------------|------------------|----------------------|------------------------|------------------------|
| $O(1)$ | Constant time | 0.000001 sec. | 0.000001 sec. | 0.000001 sec. |
| $O(\lg n)$ | Logarithmic time | 0.000007 sec. | 0.000013 sec. | 0.00002 sec. |
| $O(n)$ | Linear time | 0.0001 sec. | 0.01 sec. | 1 sec. |
| $O(n \lg n)$ | | 0.00066 sec. | 0.13 sec. | 20 sec. |
| $O(n^2)$ | Quadratic time | 0.01 sec. | 100 sec. | 278 hours |
| $O(n^3)$ | Cubic time | 1 sec. | 278 hours | 317 centuries |
| $O(2^n)$ | Exponential time | 10^{14} centuries | 10^{2995} centuries | 10^{30087} centuries |
| $O(n!)$ | Factorial time | 10^{143} centuries | 10^{35645} centuries | N/A |

FIGURE 4.2
Frequently used orders of functions and their aliases, along with their actual running time on a million-instructions-per-second machine with three input sizes: $n = 100$, 10,000, and 1,000,000.

4.2.1.1 **O-notation**

O-notation is the dominant method used to express the complexity of algorithms. It denotes the *asymptotic upper bounds* of the complexity functions. For a given function $g(n)$, the expression $O(g(n))$ (read as “big-oh of g of n ”) represents the set of functions

$$O(g(n)) = \{f(n): \text{positive constants } c \text{ and } n_0 \text{ exist such that } 0 \leq f(n) \leq cg(n) \text{ for all } n \geq n_0\}$$

A non-negative function $f(n)$ belongs to the set of functions $O(g(n))$ if there is a positive constant c that makes $f(n) \leq cg(n)$ for a sufficiently large n . We can write $f(n) \in O(g(n))$ because $O(g(n))$ is a set, but it is conventionally written as $f(n) = O(g(n))$. Readers have to be careful to note that the equality sign denotes set memberships in all kinds of asymptotic notations.

The definition of O-notation explains why lower-order terms and constant coefficients of leading terms can be ignored in complexity theory. The following are examples of legal expressions in computational theory:

$$\begin{aligned} n^2 &= O(n^2) \\ n^3 + 1000n^2 + n &= O(n^3) \\ 1000n &= O(n) \\ 20n^3 &= O(0.5n^3 + n^2) \end{aligned}$$

Figure 4.2 shows the most frequently used O-notations, their names, and the comparisons of actual running times with different values of n . The first order of functions, $O(1)$, or constant time complexity, signifies that the algorithm’s running time is independent of the input size and is the most efficient. The other O-notations are listed in their rank order of efficiency. An algorithm can be considered feasible with quadratic time complexity $O(n^2)$ for a relatively small n , but when $n = 1,000,000$, a quadratic-time algorithm takes dozens of

days to complete the task. An algorithm with a cubic time complexity may handle a problem with small-sized inputs, whereas an algorithm with exponential or factorial time complexity is virtually infeasible. If an algorithm's time complexity can be expressed with or is asymptotically bounded by a polynomial function, it has **polynomial time complexity**. Otherwise, it has **exponential time complexity**. These will be further discussed in Subsection 4.2.2.

4.2.1.2 Ω -notation and Θ -notation

Ω -notation is the inverse of O -notation. It is used to express the **asymptotic lower bounds** of complexity functions. For a given function $g(n)$, the expression $\Omega(g(n))$ (read as “big-omega of g of n ”) denotes the set of functions:

$$\Omega(g(n)) = \{f(n): \text{positive constants } c \text{ and } n_0 \text{ exist such that} \\ 0 \leq cg(n) \leq f(n) \text{ for all } n \geq n_0\}$$

From the definitions of O - and Ω -notation, the following mutual relationship holds:

$$f(n) = O(g(n)) \text{ if and only if } g(n) = \Omega(f(n))$$

Ω -notation receives much less attention than O -notation, because we are usually concerned about how much time *at most* would be spent executing an algorithm instead of the *least* amount of time spent.

Θ -notation expresses the **asymptotically tight bounds** of complexity functions. Given a function $g(n)$, the expression $\Theta(g(n))$ (read as “big-theta of g of n ”) denotes the set of functions

$$\Theta(g(n)) = \{f(n): \text{positive constants } c_1, c_2, \text{ and } n_0 \text{ exist such that} \\ 0 \leq c_1g(n) \leq f(n) \leq c_2g(n) \text{ for all } n \geq n_0\}$$

A function $f(n)$ can be written as $f(n) = \Theta(g(n))$ if there are positive coefficients c_1 and c_2 such that $f(n)$ can be squeezed between $c_1g(n)$ and $c_2g(n)$ for a sufficiently large n . Comparing the definitions of all three asymptotic notations, the following relationship holds:

$$f(n) = \Theta(g(n)) \text{ if and only if } f(n) = O(g(n)) \text{ and } f(n) = \Omega(g(n))$$

In effect, this powerful relationship is often exploited for verifying the asymptotically tight bounds of functions [Knuth 1976].

Although Θ -notation is more precise when characterizing algorithm complexity, O -notation is favored over Θ -notation for the following two reasons: (1) upper bounds are considered sufficient for characterizing algorithm complexity, and (2) it is often much more difficult to prove a tight bound than it is to prove an upper bound. In the remainder of the text, we will stick with the convention and use O -notation to express algorithm complexity.

4.2.2 Complexity classes

In the previous subsection, complexity was shown to characterize the efficiency of algorithms. In fact, complexity can also be used to characterize the problems themselves. A problem's complexity is equivalent to the time complexity of the most efficient possible algorithm. For instance, the dictionary lookup problem mentioned in the introduction of Section 4.2 has a complexity of $O(\lg n)$, the complexity of `Binary_Search` in Algorithm 4.2.

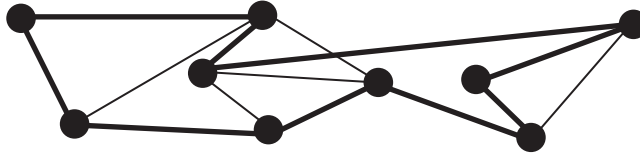
To facilitate the exploration and discussion of the complexities of various problems, those problems that share the same degree of complexity are grouped, forming complexity classes. Many complexity classes have been established in the history of computer science [Baase 1978], but in this subsection we will only discuss those that pertain to problems in the EDA applications. We will make the distinction between optimization and decision problems first, because these are key concepts within the area of complexity classes. Then, four fundamental and important complexity classes will be presented to help readers better understand the difficult problems encountered in the EDA applications.

4.2.2.1 Decision problems versus optimization problems

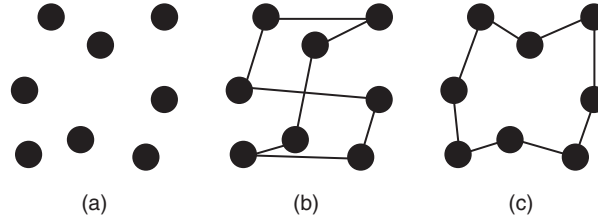
Problems can be categorized into two groups according to the forms of their answers: decision problems and optimization problems. Decision problems ask for a “yes” or “no” answer. The dictionary lookup problem, for example, is a decision problem, because the answer could only be whether the target is found or not. On the other hand, an **optimization problem** seeks for an optimized value of a target variable. For example, in a combinational circuit, a critical path is a path from an input to an output in which the sum of the gate and wire delays along the path is the largest. Finding a critical path in a circuit is an optimization problem. In this example, optimization means the *maximization* of the target variable. However, optimization can also be *minimization* in other types of optimization problems.

An example of a simple decision problem is the HAMILTONIAN CYCLE problem. The names of decision problems are conventionally given in all capital letters [Cormen 2001]. Given a set of nodes and a set of lines such that each line connects two nodes, a HAMILTONIAN CYCLE is a loop that goes through all the nodes without visiting any node twice. The HAMILTONIAN CYCLE problem asks whether such a cycle exists for a given graph that consists of a set of nodes and lines. Figure 4.3 gives an example in which a Hamiltonian cycle exists.

A famous optimization problem is the traveling salesman problem (TSP). As its name suggests, TSP aims at finding the shortest route for a salesman who needs to visit a certain number of cities in a round tour. Figure 4.4 gives a simple example of a TSP. There is also a version of the TSP as a decision problem: TRAVELING SALESMAN asks whether a route with length under a constant k exists. The optimization version of TSP is more difficult to solve than its

**FIGURE 4.3**

A graph with one HAMILTONIAN CYCLE marked with thickened lines.

**FIGURE 4.4**

(a) An example of the traveling salesman problem, with dots representing cities. (b) A non-optimal solution. (c) An optimal solution.

decision version, because if the former is solved, the latter can be immediately answered for any constant k . In fact, an optimization problem usually can be decomposed into a series of decision problems by use of a different constant as the target for each decision subproblem to search for the optimal solution. Consequently, the optimization version of a problem always has a complexity equal to or greater than that of its decision version.

4.2.2.2 The complexity classes P versus NP

The complexity class P , which stands for polynomial, consists of problems that can be solved with known polynomial-time algorithms. In other words, for any problem in the class P , an algorithm of time complexity $O(n^k)$ exists, where k is a constant. The dictionary lookup problem mentioned in Section 4.2 lies in P , because `Linear_Search` in Algorithm 4.1 has a complexity of $O(n)$.

The nondeterministic polynomial or NP complexity class involves the concept of a *nondeterministic computer*, so we will explain this idea first. A nondeterministic computer is not a device that can be created from physical components but is a conceptual tool that only exists in complexity theory. A deterministic computer, or an ordinary computer, solves problems with deterministic algorithms. The characterization of determinism as applied to an algorithm means that at any point in the process of computation the next step is always determined or uniquely defined by the algorithm and the inputs. In other words, given certain inputs and a deterministic computer, the result is always the same no matter how many times the computer executes the algorithm. By contrast, in a nondeterministic computer multiple

possibilities for the next step are available at each point in the computation, and the computer will make a *nondeterministic* choice from these possibilities, which will somehow magically lead to the desired answer. Another way to understand the idea of a nondeterministic computer is that it can execute all possible options in parallel at a certain point in the process of computation, compare them, and then choose the optimal one before continuing.

Problems in the NP complexity class have three properties:

1. They are decision problems.
2. They can be solved in polynomial time on a nondeterministic computer.
3. Their solution can be verified for correctness in polynomial time on a deterministic computer.

The TRAVELING SALESMAN decision problem satisfies the first two of these properties. It also satisfies the third property, because the length of the solution route can be calculated to verify whether it is under the target constant k in linear time with respect to the number of cities. TRAVELING SALESMAN is, therefore, an NP class problem. Following the same reasoning process, HAMILTONIAN CYCLE is also in this class.

A problem that can be solved in polynomial time by use of a deterministic computer can also definitely be solved in polynomial time on a nondeterministic computer. Thus, $P \subseteq NP$. However, the question of whether $NP = P$ remains unresolved—no one has yet been able to prove or disprove it. To facilitate this proof (or disproof), the most difficult problems in the class NP are grouped together as another complexity class, NP-complete; proving $P = NP$ is equivalent to proving $P = NP$ -complete.

4.2.2.3 The complexity class NP-complete

Informally speaking, the complexity class NP-complete (or NPC) consists of the most difficult problems in the NP class. Formally speaking, for an arbitrary problem P_a in NP and any problem P_b in the class NPC, a *polynomial transformation* that is able to transform an example of P_a into an example of P_b exists.

A polynomial transformation can be defined as follows: given two problems P_a and P_b , a *transformation* (or *reduction*) from P_a to P_b can express any example of P_a as an example of P_b . Then, the transformed example of P_b can be solved by an algorithm for P_b , and its answer can then be mapped back to an answer to the problem of P_a . A *polynomial transformation* is a transformation with a polynomial time complexity. If a polynomial transformation from P_a to P_b exists, we say that P_a is *polynomially reducible* to P_b . Now we illustrate this idea by showing that the decision problem HAMILTONIAN CYCLE is polynomially reducible to another decision problem—TRAVELING SALESMAN.

Given a graph consisting of n nodes and m lines, with each line connecting two nodes among the n nodes, a HAMILTONIAN CYCLE consists of n lines that traverse all n nodes, as in the example of Figure 4.3. This HAMILTONIAN CYCLE problem can be transformed into a TRAVELING SALESMAN problem by assigning

a distance to each pair of nodes. We assign a distance of 1 to each pair of nodes with a line connecting them. For the rest of node pairs, we assign a distance greater than 1, say, 2. With such assignments, the TRAVELING SALESMAN problem of finding whether a round tour of a total distance not greater than n exists is equal to finding a HAMILTONIAN CYCLE in the original graph. If such a tour exists, the total length of the route must be exactly n , and all the distances between the neighboring cities on the route must be 1, which corresponds to existing lines in the original graph; thus, a HAMILTONIAN CYCLE is found. This transformation from HAMILTONIAN CYCLE to TRAVELING SALESMAN is merely based on the assignments of distances, which are of polynomial time complexity—or, more precisely, quadratic time complexity—with respect to the number of nodes. Therefore the transformation is a polynomial transformation.

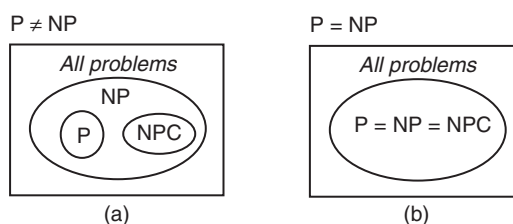
Now that we understand the concept of a polynomial transformation, we can continue discussing NP-completeness in further detail. Any problem in NPC should be polynomially reducible from any NP problem. Do we need to examine *all* NP problems if a polynomial transformation exists? In fact, a property of the NPC class can greatly simplify the proof of the NP-completeness of a problem: all problems in the class NPC are polynomially reducible to one another. Consequently, to prove that a problem P_t is indeed NPC, only two properties have to be checked:

1. The problem P_t is an NP problem, that is, P_t can be solved in polynomial time on a nondeterministic computer. This is also equivalent to showing that the solution checking of P_t can be done in polynomial time on a deterministic computer.
2. A problem already known to be NP-complete is polynomially reducible to the target problem P_t .

For example, we know that HAMILTONIAN CYCLE is polynomially reducible to TRAVELING SALESMAN. Because the former problem is an NPC problem, and TRAVELING SALESMAN is an NP problem, TRAVELING SALESMAN is, therefore, proven to be contained in the class of NPC.

Use of transformations to prove a problem to be in the NPC class relies on the assumption that there are already problems known to be NP-complete. Hence, this kind of proof is justified only if there is one problem proven to be NP-complete in another way. Such a problem is the SATISFIABILITY problem. The input of this problem is a Boolean expression in the product of sums form such as the following example: $(x_1 + x_2 + x_3)(x_2 + \bar{x}_4)(\bar{x}_1 + \bar{x}_3)(\bar{x}_2 + x_3 + x_4)$. The problem aims at assigning a Boolean value to each of the input variables x_i so that the overall product becomes true. If a solution exists, the expression is said to be *satisfiable*. Because the answer to the problem can only be true or false, SATISFIABILITY, or SAT, is a decision problem.

The NP-completeness of the SAT problem is proved with *Cook's theorem* [Cormen 2001] by showing that all NP problems can be polynomially reduced to the SAT problem. The formal proof is beyond the scope of this book [Garey

**FIGURE 4.5**

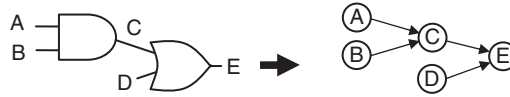
Relationship of complexity classes if (a) $P \neq NP$ or (b) $P = NP$.

1979], so we will only informally demonstrate its concept. We have mentioned that all NP problems can be solved in polynomial time on a nondeterministic computer. For an arbitrary NP problem, if we record all the steps taken on a nondeterministic computer to solve the problem in a series of statements, Cook's theorem proves that the series of statements can be polynomially transformed into a product of sums, which is in the form of an SAT problem. As a result, all NP problems can be polynomially reduced to the SAT problem; consequently, the SAT problem is NP-complete.

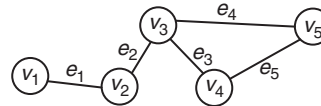
An open question in computer science is whether a problem that lies in both the P and the NPC classes exists. No one has been able to find a deterministic algorithm with a polynomial time complexity that solves any of the NP-complete problems. If such an algorithm can be found, all of the problems in NPC can be solved by that algorithm in polynomial time, because they are polynomially reducible to one another. According to the definition of NP-completeness, such an algorithm can also solve all problems in NP, making $P = NP$, as shown in Figure 4.5b. Likewise, no one has been able to prove that for any of the problems in NPC no polynomial time algorithm exists. As a result, although the common belief is that $P \neq NP$, as shown in Figure 4.5a, and decades of endeavors to tackle NP-complete problems suggest this is true, no hard evidence is available to support this point of view.

4.2.2.4 The complexity class NP-hard

Although NP-complete problems are realistically very difficult to solve, there are other problems that are even more difficult: *NP-hard* problems. The NP-hard complexity class consists of those problems at least as difficult to solve as NP-complete problems. A specific way to define an NP-hard problem is that the solution checking for an NP-hard problem cannot be completed in polynomial time. In practice, many optimization versions of the decision problems in NPC are NP-hard. For example, consider the NP-complete TRAVELING SALESMAN problem. Its optimization version, TSP, searches for a round tour going through all cities with a minimum total length. Because its solution checking requires computation of the lengths of all possible routes, which is a $O(n \cdot n!)$ procedure, with n being the number of cities, the solution definitely cannot be found in

**FIGURE 4.6**

A combinational circuit and its graph representation.

**FIGURE 4.7**

An exemplar graph.

polynomial time. Therefore, TSP, an optimization problem, belongs to the NP-hard class.

4.3 GRAPH ALGORITHMS

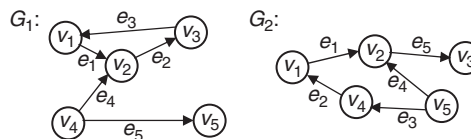
A *graph* is a mathematical structure that models pairwise relationships among items of a certain form. The abstraction of graphs often greatly simplifies the formulation, analysis, and solution of a problem. Graph representations are frequently used in the field of Electronic Design Automation. For example, a combinational circuit can be efficiently modeled as a *directed graph* to facilitate structure analysis, as shown in Figure 4.6.

Graph algorithms are algorithms that exploit specific properties in various types of graphs [Even 1979; Gibbons 1985]. Given that many problems in the EDA field can be modeled as graphs, efficient graph algorithms can be directly applied or slightly modified to address them. In this section, the terminology and data structures of graphs will first be introduced. Then, some of the most frequently used graph algorithms will be presented.

4.3.1 Terminology

A graph G is defined by two sets: a vertex set V and an edge set E . Customarily, a graph is denoted with $G(V, E)$. Vertices can also be called *nodes*, and edges can be called *arcs* or *branches*. In this chapter, we use the terms *vertices* and *edges*.

Figure 4.7 presents a graph G with $V = \{v_1, v_2, v_3, v_4, v_5\}$ and $E = \{e_1, e_2, e_3, e_4, e_5\}$. The two vertices connected by an edge are called the edge's *endpoints*. An edge can also be characterized by its two endpoints, u and v , and denoted as (u, v) . In the example of Figure 4.7, $e_1 = (v_1, v_2)$, $e_2 = (v_2, v_3)$, etc. If there is an edge e connecting u and v , the two vertices u and v are *adjacent* and edge e is

**FIGURE 4.8**

Two examples of directed graphs.

incident with u (and also with v). The *degree* of a vertex is equal to the number of edges incident with it.

A *loop* is an edge that starts and ends at the same vertex. If plural edges are incident with the same two vertices, they are called *parallel edges*. A graph without loops and parallel edges is called a *simple graph*. In most discussions of graphs, only simple graphs are considered, and, thus, a graph implicitly means a simple graph. A graph without loops but with parallel edges is known as a *multigraph*.

The number of vertices in a graph is referred to as the *order* of the graph, or simply $|V|$. Similarly, the *size* of a graph, denoted as $|E|$, refers to its number of edges. It is worth noting that inside asymptotic notations, such as O and Θ , and *only* inside them, $|V|$ and $|E|$ can be simplified as V and E . For example, $O(|V| + |E|)$ can be expressed as $O(V + E)$.

A *path* in a graph is a sequence of alternating vertices and edges such that for each vertex and its next vertex in the sequence, the edge between these vertices connects them. The *length* of a path is defined as the number of edges in a path. For example, in Figure 4.7, $\langle v_5, e_4, v_3, e_3, v_4 \rangle$ is a path with a length of two. A path in which the first and the last vertices are the same is called a *cycle*. $\langle v_5, e_4, v_3, e_3, v_4, e_5, v_5 \rangle$ is a cycle in Figure 4.7. A path, in which every vertex appears once in the sequence is called a *simple* path. The word “simple” is often omitted when this term is used, because we are only interested in simple paths most of the time.

The terms defined so far are for *undirected* graphs. In the following, we introduce the terminology for *directed* graphs. In a *directed* graph, every edge has a direction. We typically use arrows to represent directed edges as shown in the examples in Figure 4.8. For an edge $e = (u, v)$ in a directed graph, u and v cannot be freely exchanged. The edge e is directed from u to v , or equivalently, *incident from u* and *incident to v* . The vertex u is the *tail* of the edge e ; v is the *head* of the edge e . The degree of a vertex in a directed graph is divided into the *in-degree* and the *out-degree*. The *in-degree* of a vertex is the number of edges incident *to* it, whereas the *out-degree* of a vertex is the number of edges incident *from* it. For the example of G_2 in Figure 4.8, the in-degree of v_2 is 2 and its out-degree is 1.

The definitions of paths and cycles need to be revised as well for a directed graph: every edge in a path or a cycle must be preceded by its tail and followed by its head. For example, $\langle v_4, e_4, v_2, e_2, v_3 \rangle$ in G_1 of Figure 4.8 is a path and $\langle v_1, e_1, v_2, e_2, v_3, e_3, v_1 \rangle$ is a cycle, but $\langle v_4, e_4, v_2, e_1, v_1 \rangle$ is not a path.

If a vertex u appears before another vertex v in a path, u is v 's *predecessor* on that path and v is u 's *successor*. Notice that there is no cycle in G_2 . Such directed graphs without cycles are called *directed acyclic graphs* or *DAGs*. DAGs are powerful tools used to model combinational circuits, and we will dig deeper into their properties in the following subsections.

In some applications, we can assign values to the edges so that a graph can convey more information related to the edges other than their connections. The values assigned to edges are called their *weights*. A graph with weights assigned to edges is called a *weighted graph*. For example, in a DAG modeling of a combinational circuit, we can use weights to represent the time delay to propagate a signal from the input to the output of a logic gate. By doing so, critical paths can be conveniently determined by standard graph algorithms.

4.3.2 Data structures for representations of graphs

Several data structures are available to represent a graph in a computer, but none of them is categorically better than the others [Aho 1983; Tarjan 1987]. They all have their own advantages and disadvantages. The choice of the data structure depends on the algorithm [Hopcroft 1973].

The simplest data structure for a graph is an *adjacency matrix*. For a graph $G = (V, E)$, a $|V| \times |V|$ matrix A is needed. $A_{ij} = 1$ if $(v_i, v_j) \in E$, and $A_{ij} = 0$ if $(v_i, v_j) \notin E$. For an undirected graph, the adjacency matrix is symmetrical, because the edges have no directions. Figure 4.9 shows the adjacency matrices for the graph in Figure 4.7 and G_2 in Figure 4.8.

One of the strengths of the use of an adjacency matrix is that it can easily represent a weighted graph by changing the ones in the matrix to the edges' respective weights. However, the weight cannot be a zero in this representation (otherwise we cannot differentiate zero-weight edge from "no connection" between two vertices). Also, an adjacency matrix requires exactly $\Theta(V^2)$ space. For a *dense* graph for which $|E|$ is close to $|V|^2$, this could be a memory-efficient representation. However, if the graph is *sparse*, that is, $|E|$ is much smaller than $|V|^2$, most of the entries in the adjacency matrix would be zeros, resulting in a waste of memory.

A sparse graph is better represented with an *adjacency list*, which consists of an array of size $|V|$, with the i th element corresponding to the vertex v_i . The i th element points to a *linked list* that stores those vertices adjacent to v_i .

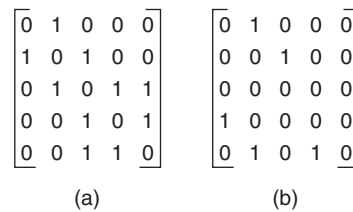
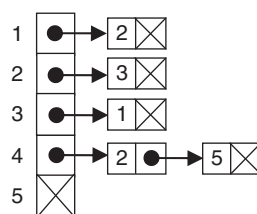


FIGURE 4.9

The adjacency matrices: (a) for Figure 4.7. (b) for G_2 in Figure 4.8.

**FIGURE 4.10**

The adjacency list for G_1 of Figure 4.8.

in an undirected graph. For a directed graph, any vertex v_j in the linked list of the i th element satisfies the condition $(v_i, v_j) \in E$. The adjacency list for G_1 in Figure 4.8 is shown in Figure 4.10.

4.3.3 Breadth-first search and depth-first search

Many graph algorithms rely on efficient and systematic traversals of vertices and edges in the graph. The two simplest and most commonly used traversal methods are *breadth-first search* and *depth-first search*, which form the basis for many graph algorithms. We will examine their generic structures and point out some important applications.

4.3.3.1 Breadth-first search

Breadth-first search (BFS) is a systematic means of visiting vertices and edges in a graph. Given a graph G and a specific **source** vertex s , the BFS searches through those vertices adjacent to s , then searches the vertices adjacent to those vertices, and so on. The routine stops when BFS has visited all vertices that are reachable from s . The phenomenon that the vertices closest to the source s are visited earlier in the search process gives this search its name. Several procedures can be executed when visiting a vertex. The function BFS in Algorithm 4.3 adopts two of the most frequently used procedures: building a *breadth-first tree* and calculating the distance, which is the minimum length of a path, from the source s to each reachable vertex.

Algorithm 4.3 Breadth-first Search Algorithm

BFS (Graph G , Vertex s)

1. FIFO_Queue $Q = \{s\}$;
2. **for** (each $v \in V$) **do**
3. $v.\text{visited} = \text{false}$; // visited by BFS
4. $v.\text{distance} = \infty$; // distance from source s
5. $v.\text{predecessor} = \text{NIL}$; // predecessor of v
6. **end for**
7. $s.\text{visited} = \text{true}$;


```

8. s.distance = 0;
9. while ( $Q \neq \emptyset$ ) do
10.   Vertex  $u = \text{Dequeue}(Q)$ ;
11.   for (each  $(u, w) \in E$ ) do
12.     if ( $\neg(w.\text{visited})$ )
13.        $w.\text{visited} = \text{true}$ ;
14.        $w.\text{distance} = u.\text{distance} + 1$ ;
15.        $w.\text{predecessor} = u$ ;
16.        $\text{Enqueue}(Q, w)$ ;
17.     end if
18.   end for
19. end while

```

The function `BFS` implements breadth-first search with a queue Q . The queue Q stores the indices of, or the links to, the visited vertices whose adjacent vertices have not yet been examined. The first-in first-out (FIFO) property of a queue guarantees that `BFS` visits every reachable vertex once, and all of its adjacent vertices are explored in a breadth-first fashion. Because each vertex and edge is visited at most once, the time complexity of a generic BFS algorithm is $O(V + E)$, assuming the graph is represented by an adjacency list.

Figure 4.11 shows a graph produced by the `BFS` in Algorithm 4.3 that also indicates a breadth-first tree rooted at v_1 and the distances of each vertex to v_1 . The distances of v_7 and v_8 are infinity, which indicates that they are *disconnected* from v_1 . In contrast, subsets of a graph in which the vertices are connected to one another and to which no additional vertices are connected, such as the set from v_1 to v_6 in Figure 4.11, are called *connected components* of the graph. One of the applications of `BFS` is to find the connected components of a graph. The attributes `distance` and `predecessors` indicate the lengths and the routes of the shortest paths from each vertex to the vertex v_1 . A BFS algorithm

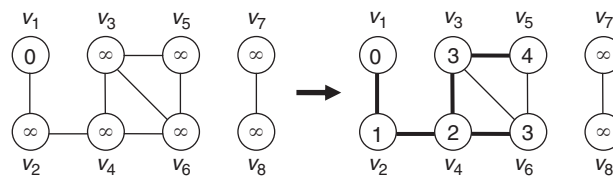


FIGURE 4.11

Applying `BFS` on an undirected graph with source v_1 . The left is the graph after line 8 and the right shows the graph after the completion of the `BFS`. Numbers in the vertices are their distances to the source v_1 . Thick edges are breadth-first tree edges.

can also compute the shortest paths and their lengths from a source vertex to all other vertices in an *unweighted* graph. The calculation of the shortest paths in a weighted graph will be discussed in Subsection 4.3.6.

4.3.3.2 *Depth-first search*

While BFS traverses a graph in a breadth-first fashion, *depth-first search* (DFS) explores the graph in an opposite manner. From a predetermined source vertex s , DFS traverses the vertex as deep as possible along a path before backtracking, just as the name implies. The recursive function `DFSPrototype`, shown in Algorithm 4.4, is the basic structure for a DFS algorithm.

Algorithm 4.4 A Prototype of the Depth-first Search Algorithm

```
DFSPrototype(Vertex  $v$ )
1. // Pre-order process on  $v$ ;
2. mark  $v$  as visited;
3. for (each unvisited vertex  $u$  adjacent to  $v$ )
4.   DFSPrototype( $u$ );
5.   // In-order process on  $v$ ;
6. end for
7. // Post-order process on  $v$ 
```

The terms *pre-order*, *in-order*, and *post-order* processes on the lines 1, 5, and 7 in Algorithm 4.4 refer to the traversal patterns on a conceptual tree formed by all the vertices in the graph. DFS performs a pre-order process on all the vertices in the exact same order as a pre-order tree traversal in the resulting “*depth-first forest*.” This is also the case for in-order and post-order processes. The functionality of these processes, which will be tailor-designed to an application, is the basis of DFS algorithms. The function `DFS` in Algorithm 4.5 provides an example of a post-order process.

Algorithm 4.5 A Complete Depth-first Search Algorithm

```
DFS(Graph  $G$ )
1. for (each vertex  $v \in V$ ) do
2.    $v$ .visited = false;
3.    $v$ .predecessor = NIL;
4. end for
5.  $time = 0$ ;
6. for (each vertex  $v \in V$ )
7.   if ( $\neg v$ .visited)
8.     DFSVisit( $v$ );
```

```

9.   end if
10. end for
DFSVisit(Vertex  $v$ )
1.   $v.\text{visited} = \text{true};$ 
2.  for (each  $(v, u) \in E$ )
3.    if ( $\neg(u.\text{visited})$ ) do
4.       $u.\text{predecessor} = v;$ 
5.      DFSVisit( $u$ );
6.    end if
7.  end for
8.   $\text{time} = \text{time} + 1;$ 
9.   $v.\text{PostOrderTime} = \text{time};$ 

```

Notice that it is guaranteed that every vertex will be visited by lines 6 and 7 in DFS. This is another difference between DFS and BFS. For most applications of DFS, it is preferred that all vertices in the graph be visited. As a result, a *depth-first forest* is formed instead of a tree. Moreover, because each vertex and edge is explored exactly once, the time complexity of a generic DFS algorithm is $O(V + E)$ assuming the use of an adjacency list.

Figure 4.12 demonstrates a directed graph on which $\text{DFS}(G_1)$ is executed. The `PostOrderTimes` of all vertices and the tree edges of a depth-first forest, which is constructed from the `predecessor` of each vertex, are produced as the output. `PostOrderTimes` have several useful properties. For example, the vertices with a lower post-order time are never predecessors of those with a higher post-order time on any path. The next subsection uses this property for sorting the vertices of a DAG. In Subsection 4.3.5, we will introduce some important applications of the depth-first forest.

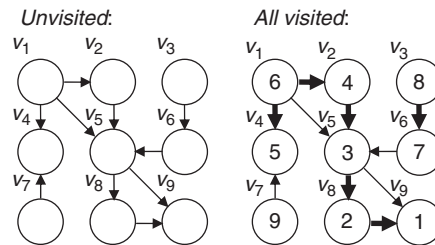
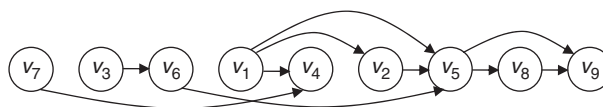


FIGURE 4.12

Applying DFS on a directed graph G_1 . The numbers in the vertices are their `PostOrderTimes`. Thickened edges show how a depth-first forest is built.

**FIGURE 4.13**

A topological sort of the graph in Figure 4.12.

4.3.4 Topological sort

A *topological sort* is a linear ordering of vertices in a **directed acyclic graph** (DAG). Given a DAG $G = (V, E)$, a topological sort algorithm returns a sequence of vertices in which the vertices never come before their predecessors on any paths. In other words, if $(u, v) \in E$, v never appears before u in the sequence. A topological sort of a graph can be represented as a horizontal line of ordered vertices, such that all edges point only to the right (Figure 4.13).

DAGs are used in various applications to show precedence among events. In the EDA industry, DAGs are especially useful because they are capable of modeling the input-output relationships of combinational circuits, as shown in Figure 4.6. To effectively simulate a combinational circuit with EDA tools, inputs of a gate should usually be examined before the output is analyzed. A topological sort of a DAG provides an appropriate ordering of gates for simulations.

The simple algorithm in Algorithm 4.6 topologically sorts a DAG by use of the depth-first search. Note that line 2 in Algorithm 4.6 should be embedded into line 9 of the function `DFSVisit` in Algorithm 4.5 so that the complexity of the function `TopologicalSortByDFS` remains $O(V + E)$. The result of running `TopologicalSortByDFS` on the graph in Figure 4.12 is shown in Figure 4.13. The vertices are indeed topologically sorted.

Algorithm 4.6 A Simple DFS-based Topological Sort Algorithm

`TopologicalSortByDFS(Graph G)`

1. call `DFS(G)` in Algorithm 4.5;
 2. as `PostOrderTime` of each vertex v is computed, insert v onto the front of a linked list //;
 3. **return** //;
-

Another intuitive algorithm, shown in Algorithm 4.7, can sort a DAG topologically without the overhead of recursive functions typically found in DFS. With careful programming, it has a linear time complexity $O(V + E)$. This version of a topological sort is also superior because it can detect cycles in a directed graph. One application of this feature is efficiently finding feedback loops in a circuit, which should not exist in a combinational circuit.

Algorithm 4.7 A Topological Sort Algorithm that can Detect Cycles

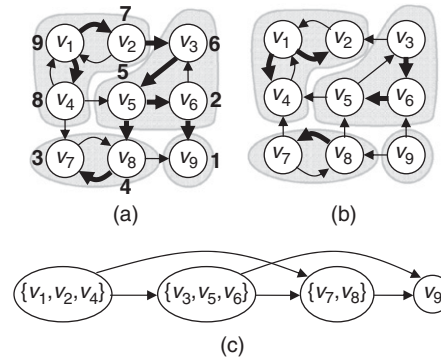
TopologicalSort(Graph G)

1. FIFO_Queue $Q = \{\text{vertices with in-degree } 0\}$;
2. LinkedList $ll = \emptyset$;
3. **while** (Q is not empty) **do**
4. Vertex $v = \text{Dequeue}(Q)$;
5. insert v into ll ;
6. **for** (each vertex u such that $(v, u) \in E$) **do**
7. remove (v, u) from E ;
8. **if** (in-degree of u is 0) Enqueue(Q, u);
9. **end for**
10. **end while**
11. **if** ($E \neq \emptyset$) **return** “G has cycles”;
12. **else return** ll ;

4.3.5 Strongly connected component

A connected component in an undirected graph has been defined in Subsection 4.3.3.1. For a directed graph, connectivity is further classified into “*strong connectivity*” and “*weak connectivity*.” A directed graph is *weakly* connected if all vertices are connected provided all directed edges are replaced as undirected edges. For a *strongly connected* directed graph, every vertex must be reachable from every other vertex. More precisely, for any two vertices u and v in a strongly connected graph, there exists a path from u to v , as well as a path from v to u . A *strongly connected component* (SCC) in a directed graph is a subset of the graph that is strongly connected and is maximal in the sense that no additional vertices can be included in this subset while still maintaining the property of strong connectivity. Figure 4.14a shows a weakly connected graph with four strongly connected components. As an SCC consisting of more than one vertex must contain cycles, it follows naturally that a directed *acyclic* graph has no SCCs that consist of more than one vertex.

The algorithm used to extract SCCs, SCC in Algorithm 4.8, requires the knowledge of the *transpose* of a directed graph (line 2). A transpose of a directed graph G , G^T , contains the same vertices of G , but the directed edges are reversed. Formally speaking, for $G = (V, E)$, $G^T = (V, E^T)$ with $E^T = \{(u, v) : (v, u) \in E\}$. Transposing a graph incurs a linear time complexity $O(V + E)$, which preserves the efficiency of the algorithm for finding SCCs.

**FIGURE 4.14**

(a) A directed graph G after running DFS with depth-first tree edges thickened. Post-order times are labeled beside each vertex and SCC regions are shaded. (b) The graph G^T , the transpose of G , after running SCC in Algorithm 4.8 (c) Finding SCCs in G as individual vertices result in a DAG.

Algorithm 4.8 An Algorithm to Extract SCCs from a Directed Graph

SCC(Graph G)

1. call DFS(G) in Algorithm 4.5 for PostOrderTime;
 2. $G^T = \text{transpose}(G)$;
 3. call DFS(G^T), replacing line 6 of DFS with a procedure examining vertices in order of decreasing PostOrderTime;
 4. **return** different trees in depth-first forest built in DFS(G^T) as separate SCCs;
-

SCC is simple: a DFS, then a transpose, then another DFS. It is also efficient because DFS and transpose incur only a linear time complexity, resulting in a time complexity of $O(V + E)$. Figure 4.14 gives an example of running SCC on a graph G . The four SCCs are correctly identified by the four depth-first trees in G^T . Moreover, if we view an SCC as a single vertex, the resultant graph, shown in Figure 4.14, is a DAG. We also observe that examining vertices in a descending order of the post-order times in DFS is equivalent to visiting the resultant SCCs in a topologically sorted order.

If we model a sequential circuit as a directed graph where vertices represent registers and edges represent combinational signal flows between registers, extracting SCCs from the graph identifies clusters of registers, each of which includes a set of registers with strong functional dependencies among themselves. Extracting SCCs also enables us to model each SCC as a single element, which greatly facilitates circuit analysis because the resultant graph is a DAG.

4.3.6 Shortest and longest path algorithms

Given a combinational circuit in which each gate has its own delay value, suppose we want to find the critical path—that is, the path with the longest delay—from an input to an output. A trivial solution is to explicitly evaluate all paths from the input to the output. However, the number of paths can grow exponentially with respect to the number of gates. A more efficient solution exists: we can model the circuit as a directed graph whose edge weights are the delays of the gates. The *longest path algorithm* can then give us the answer more efficiently.

In this subsection, we present various shortest and longest path algorithms. Not only can they calculate the delays of critical paths, but they also can be applied to other EDA problems, such as finding an optimal sequence of state transitions from the starting state to the target state in a state transition diagram. In the *shortest-path problem* or the *longest-path problem*, we are given a **weighted, directed** graph. The weight of a path is defined as the sum of the weights of its constituent edges. The goal of the shortest-/longest-path problem is to find the path from a source vertex s to a destination vertex d with minimum/maximum weight. Three algorithms are capable of finding the shortest paths from a source to all other vertices, each of which works on the graph with different constraints. First, we will present a simple algorithm used to solve the shortest-path problem on DAGs. *Dijkstra's algorithm* [Dijkstra 1959], which functions on graphs with non-negative weights, will then be presented. Finally, we will introduce a more general algorithm that can be applied to all types of directed graphs—the *Bellman-Ford algorithm* [Bellman 1958]. On the basis of these algorithms' concepts, we will demonstrate how to modify them to apply to longest-path problems.

4.3.6.1 Initialization and relaxation

Before explaining these algorithms, we first introduce two basic techniques used by all the algorithms in this subsection: initialization and relaxation.

Before running a shortest-path algorithm on a directed graph $G = (V, E)$, we must be given a source vertex s and the weight of each edge $e \in E$, $w(e)$. Also, two attributes must be stored for each vertex $v \in V$: the **predecessor** $pre(v)$ and the **shortest-path estimate** $est(v)$. The predecessor $pre(v)$ records the predecessor of v on the shortest path, and $est(v)$ is the current estimation of the weight of the shortest path from s to v . The procedure in Algorithm 4.9, known as *initialization*, initializes $pre(v)$ and $est(v)$ for all vertices.

Algorithm 4.9 Initialization Procedure for Shortest-path Algorithms

Initialize(graph G , Vertex s)

1. **for** (each vertex $v \in V$) **do**
 2. $pre(v) = \text{NIL}$; // predecessor
 3. $est(v) = \infty$; // shortest-path estimate
 4. **end for**
 5. $est(s) = 0$;
-

The other common procedure, **relaxation**, is the kernel of all the algorithms presented in this subsection. The *relaxation* of an edge (u, v) is the process of determining whether the shortest path to v found so far can be shortened or relaxed by taking a path through u . If the shortest path is, indeed, improved by use of this procedure, $pre(v)$ and $est(v)$ will be updated. Algorithm 4.10 shows this important procedure.

Algorithm 4.10 Relaxation Procedure for Shortest-path Algorithms

Relax(Vertex u , Vertex v)

1. **if** ($est(v) > est(u) + w(u, v)$) **do**
 2. $est(v) = est(u) + w(u, v)$;
 3. $pre(v) = u$;
 4. **end if**
-

4.3.6.2 Shortest path algorithms on directed acyclic graphs

DAGs are always easier to manipulate than the general directed graphs, because they have no cycles. By use of a topological sorting procedure, as shown in Algorithm 4.11, this $\Theta(V + E)$ algorithm calculates the shortest paths on a DAG with respect to a given source vertex s .

The function DAGShortestPaths, used in Algorithm 4.11, sorts the vertices topologically first; in line 4, each vertex is visited in the topologically sorted order. As each vertex is visited, the function relaxes all edges incident from it. The shortest paths and their weights are then available in $pre(v)$ and $est(v)$ of each vertex v . Figure 4.15 gives an example of running DAGShortestPaths on a DAG. Notice that the presence of negative weights in a graph does not affect the correctness of this algorithm.

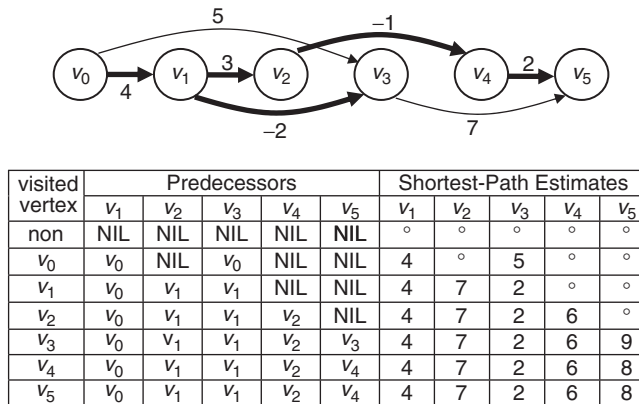
Algorithm 4.11 A Shortest-path Algorithm for DAGs

DAGShortestPaths(Graph G , vertex s)

1. topologically sort the vertices of G ;
 2. Initialize(G, s);
 3. **for** (each vertex u in topological sorted order)
 4. **for** (each vertex v such that $(u, v) \in E$)
 5. Relax(u, v);
 6. **end for**
 7. **end for**
-

4.3.6.3 Dijkstra's algorithm

Dijkstra's algorithm solves the shortest-path problem for any weighted, directed graph with **non-negative** weights. It can handle graphs consisting of cycles,

**FIGURE 4.15**

The upper part is a DAG with its shortest paths shown in thickened edges, and the lower part is the changes of predecessors and shortest-path estimates when different vertices are visited in line 3 of the function `DAGShortestPaths`.

but negative weights will cause this algorithm to produce incorrect results. Consequently, we assume that $w(e) \geq 0$ for all $e \in E$ here.

The pseudocode in Algorithm 4.12 shows Dijkstra's algorithm. The algorithm maintains a priority queue `minQ` that is used to store the unprocessed vertices with their shortest-path estimates $est(v)$ as key values. It then repeatedly extracts the vertex u which has the minimum $est(u)$ from `minQ` and relaxes all edges incident from u to any vertex in `minQ`. After one vertex is extracted from `minQ` and all relaxations through it are completed, the algorithm will treat this vertex as processed and will not touch it again. Dijkstra's algorithm stops either when `minQ` is empty or when every vertex is examined exactly once.

Algorithm 4.12 Dijkstra's shortest-path algorithm

Dijkstra(Graph G , Vertex s)

1. Initialize(G , s);
 2. Priority_Queue `minQ` = {all vertices in V };
 3. **while** (`minQ` $\neq \emptyset$) **do**
 4. Vertex u = ExtractMin(`minQ`); // minimum $est(u)$
 5. **for** (each $v \in \text{minQ}$ such that $(u, v) \in E$)
 6. Relax(u , v);
 7. **end for**
 8. **end while**
-

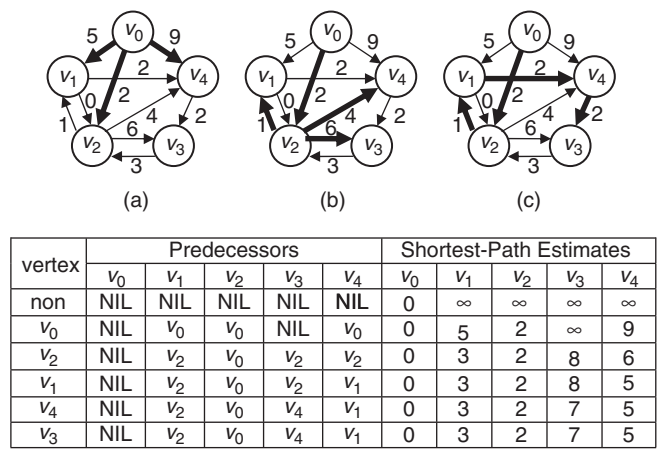


FIGURE 4.16 An example of Dijkstra’s algorithm: (a), (b), and (c) respectively show the edges belonging to the shortest paths when v_0 , v_2 , and v_3 are visited. The table exhibits the detailed data when each vertex is visited.

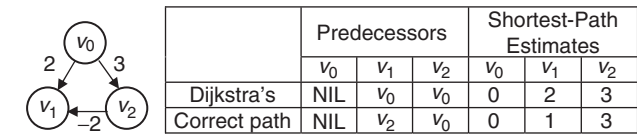


FIGURE 4.17 Running Dijkstra’s algorithm on a graph with negative weights causes incorrect results on v_1 .

Dijkstra’s algorithm works correctly, because all edge weights are non-negative, and the vertex with the least shortest-path estimate is always chosen. In the first iteration of the `while` loop in lines 3 through 7, the source s is chosen and its adjacent vertices have their $est(v)$ set to $w((s, v))$. In the second iteration, the vertex u with minimal $w((s, u))$ will be selected; then those edges incident from u will be relaxed. Clearly, there exists no shorter path from s to u than the single edge (s, u) , because all weights are not negative, and any path traced that uses an intermediate vertex is longer. Continuing this reasoning brings us to the conclusion that the algorithm, indeed, computes the shortest paths.

Figure 4.16 illustrates the execution of Dijkstra’s algorithm on a directed graph with non-negative weights and containing cycles. However, a small example in Figure 4.17 shows that Dijkstra’s algorithm fails to find the shortest paths when negative weights exist.

Dijkstra’s algorithm necessitates the use of a priority queue that supports the operations of extracting a minimum element and decreasing keys. A linear array can be used, but its complexity will be as much as $O(V^2 + E) = O(V^2)$. If a more

efficient data structure, such as a *binary* or *Fibonacci heap* [Moore 1959], is used to implement the priority queue, the complexity can be reduced.

4.3.6.4 The Bellman-Ford algorithm

Cycles should never appear in a shortest path. However, if there exist negative-weight cycles, a shortest path can have a weight of $-\infty$ by circling around negative-weight cycles infinitely many times. Therefore, negative-weight cycles should be avoided before finding the shortest paths. In general, we can categorize cycles into three types according to their weights: negative-weight, zero-weight, and positive-weight cycles. Positive-weight cycles would not appear in any shortest paths and thus will never be threats. Zero-weight cycles are unwelcome in most applications, because we generally want a shortest path to have not only a minimum weight, but also a minimum number of edges.

Because a shortest path should not contain cycles, it should traverse every vertex at most once. It follows that in a directed graph $G = (V, E)$, the maximum number of edges a shortest path can have is $|V| - 1$, with all the vertices visited once. The *Bellman-Ford algorithm* takes advantage of this observation and relaxes all the edges $(|V| - 1)$ times. Although this strategy is time-consuming, with a runtime of $O((|V| - 1) \times |E|) = O(VE)$, it helps the algorithm handle more general cases, such as graphs with negative weights. It also enables the discovery of negative-weight cycles.

The pseudocode of the Bellman-Ford algorithm is shown in Algorithm 4.13. The negative-weight cycles are detected in lines 5 through 7. They are identified on the basis of the fact that if any edge can still be relaxed after $(|V| - 1)$ times of relaxations (line 6), then a shortest path with more than $(|V| - 1)$ edges exists; therefore, the graph contains negative-weight cycles.

Algorithm 4.13 Bellman-Ford algorithm

Bellman-Ford(Graph G , Vertex s)

1. Initialize(G, s);
 2. **for** ($counter = 1$ to $|V| - 1$)
 3. **for** (each edge $(u, v) \in E$)
 4. Relax(u, v);
 5. **end for**
 6. **end for**
 7. **for** (each edge $(u, v) \in E$)
 8. **if** ($est(v) > est(u) + w(u, v)$)
 9. report “negative-weight cycles exist”;
 10. **end if**
 11. **end for**
-

4.3.6.5 The longest-path problem

The longest-path problem can be solved by use of a modified version of the shortest-path algorithm. We can multiply the weights of the edges by -1 and feed the graph into either the shortest-path algorithm for DAGs or the Bellman-Ford algorithm. We cannot use Dijkstra's algorithm, which cannot handle graphs with negative-weight edges. Rather than finding the shortest path, these algorithms discover the longest path. If we do not want to alter any attributes in the graph, we can alter the algorithm by initializing the value of $est(v)$ to $-\infty$ instead of ∞ , as shown in the `Initialize` procedure of Algorithm 4.9, and changing a line in the `Relaxation` procedure of Algorithm 4.10 from:

```

1. if ( $est(v) > est(u) + w(u, v)$ ){
to
1. if ( $est(v) < est(u) + w(u, v)$ ){

```

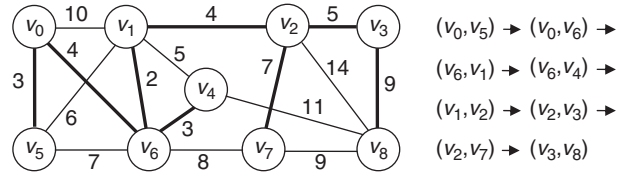
Again, this modification cannot be applied to Dijkstra's algorithm, because positive-weight cycles should be avoided in the longest paths, but avoiding them is difficult, because all or most weights are positive in most applications. As a result, the longest-path version of the Bellman-Ford algorithm, which can detect positive-weight cycles, is typically favored for use. If we want to find the longest *simple* paths in those graphs where positive cycles exist, then no efficient algorithm yet exists, because this problem is NP-complete.

4.3.7 Minimum spanning tree

Spanning trees are defined on **connected, undirected** graphs. Given a graph $G = (V, E)$, a spanning tree connects all of the vertices in V by use of some edges in E without producing cycles. A spanning tree has exactly $(|V| - 1)$ edges. For example, the thickened edges shown in Figure 4.18 form a spanning tree. The *tree weight* of a spanning tree is defined as the sum of the weights of the tree edges. There would be many spanning trees in a connected, weighted graph with different tree weights. The *minimum spanning tree (MST) problem* searches for a spanning tree whose tree weight is minimized. The MST problem can model the construction of a power network with a minimum wire length in an integrated circuit. It can also model the clock network, which connects the clock source to each terminal with the least number of clock delays. In this subsection, we present an algorithm for the MST problem, *Prim's algorithm* [Prim 1957].

Prim's algorithm builds an MST by maintaining a set of vertices and edges. This set initially includes a starting vertex. The algorithm then adds edges (along with vertices) one by one to the set. Each time the edge closest to the set—with the least edge weight to any of the vertices in the set—is added. After the set contains all the vertices, the edges in the set form a minimum spanning tree.

The pseudocode of Prim's algorithm is given in Algorithm 4.14. The function `PrimMST` uses a priority queue `minQ` to store those vertices not yet included in

**FIGURE 4.18**

An example of an MST returned by Prim's algorithm. The MST consists of the thickened edges. The order of choices is shown on the right.

the partial MST. Every vertex in minQ is keyed with its minimum edge weight to the partial MST. In line 7, the vertex with the minimum key is extracted from minQ , and the keys of its adjacent vertices are updated accordingly, as shown in lines 8 through 11. The parameter `predecessor` refers to MST edges.

Algorithm 4.14 Prim's MST algorithm

PrimMST(Graph G)

1. Priority_Queue $\text{minQ} = \{\text{all vertices in } V\}$;
 2. for(each vertex $u \in \text{minQ}$) $u.\text{key} = \infty$;
 3. randomly select a vertex r in V as root;
 4. $r.\text{key} = 0$;
 5. $r.\text{predecessor} = \text{NIL}$;
 6. **while** ($\text{minQ} \neq \emptyset$) **do**
 7. Vertex $u = \text{ExtractMin}(\text{minQ})$;
 8. **for** (each vertex v such that $(u, v) \in E$) **do**
 9. **if** ($v \in \text{minQ}$ and $w(u, v) < v.\text{key}$) **do**
 10. $v.\text{predecessor} = u$;
 11. $v.\text{key} = w(u, v)$;
 12. **end if**
 13. **end for**
 14. **end while**
-

Like Dijkstra's algorithm, the data structure of minQ determines the runtime of Prim's algorithm. PrimMST has a time complexity of $O(V^2 + E)$ if minQ is implemented with a linear array. However, less time complexity can be achieved by use of a more sophisticated data structure.

Figure 4.18 shows an example in which Prim's MST algorithm selects the vertex v_0 as the starting vertex. In fact, an MST can be built from any starting vertex. Moreover, an MST is not necessarily unique. For example, if the edge (v_7, v_8) replaces the edge (v_3, v_8) , as shown in Figure 4.18, the new set of edges still forms an MST.

The strategy used by Prim's algorithm is actually very similar to that of Dijkstra's shortest-path algorithm. Dijkstra's algorithm implicitly keeps a set of processed vertices and chooses an unprocessed vertex that has a minimum shortest-path estimate at the moment to be the next target of relaxation. This strategy follows the principle of a *greedy algorithm*. This concept will be explained in Subsection 4.4.1.

4.3.8 Maximum flow and minimum cut

4.3.8.1 Flow networks and the maximum-flow problem

A **flow network** is a variant of *connected, directed* graphs that can be used to model physical flows in a network of terminals, such as water coursing through interconnecting pipes or electrical currents flow through a circuit. In a flow network $G = (V, E)$, every edge $(u, v) \in E$ has a non-negative *capacity* $c(u, v)$ that indicates the quantity of flow this edge can hold. If $(u, v) \notin E$, $c(u, v) = 0$. There are two special vertices in a flow network, the *source* s and the *sink* t . Every flow must start at the source s and end at the sink t . Hence, there is no edge incident to s and neither an edge leaving t . For convenience, we assume that every vertex lies on some path from the source to the sink. Every edge (u, v) in a flow network has another attribute, *flow* $f(u, v)$, which is a real number that satisfies the following three properties:

Capacity constraint: For every edge $(u, v) \in E$, $f(u, v) \leq c(u, v)$.

Skew symmetry: For every flow $f(u, v)$, $f(u, v) = -f(v, u)$.

Flow conservation: For all vertices in V , the flows entering it are equal to the flows exiting it, making the *net flow* of every vertex zero. There are two exceptions to this rule: the source s , which generates the flow, and the sink t , which absorbs the flow. Therefore, for all vertices $u \in V - \{s, t\}$, the following equality holds:

$$\sum_{v \in V} f(u, v) = 0$$

Notice that the flow conservation property corresponds to Kirchhoff's Current Law, which describes the principle of conservation in electric circuits. Therefore, the flow networks can naturally model electric currents.

The *value* of a flow f is defined as:

$$|f| = \sum_{v \in V} f(s, v)$$

which is the total flow out of the source. In a **maximum-flow problem**, the goal is to find a flow with the maximal value in a flow network. Figure 4.19 is an example of a flow network G with a flow f . The values shown on every edge (u, v) are $f(u, v)/c(u, v)$. In this example, $|f| = 19$, but it is not a maximum flow, because we can push more flow into the path $s \rightarrow v_2 \rightarrow v_3 \rightarrow t$.

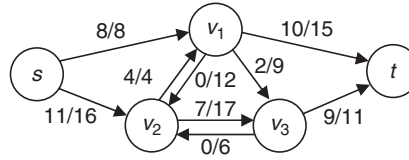


FIGURE 4.19

A flow network G with a flow $f = 19$. The flow and the capacity of each edge are denoted as $f(u, v)/c(u, v)$.

4.3.8.2 Augmenting paths and residual networks

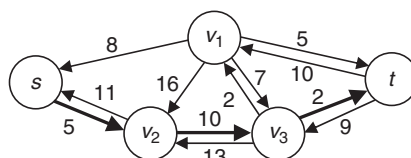
The path $s \rightarrow v_2 \rightarrow v_3 \rightarrow t$ in Figure 4.19 can accommodate more flow and, thus, it can enlarge the value of the total flow. Such paths from the source to the sink are called **augmenting paths**. An intuitive maximum-flow algorithm operates by iteratively finding augmenting paths and then augmenting a corresponding flow until there is no more such path. However, finding these augmenting paths on flow networks is neither easy nor effective. **Residual networks** are hence created to simplify the process of finding augmenting paths.

In the flow network $G = (V, E)$ with a flow f , for every edge $(u, v) \in E$ we define its *residual capacity* $c_f(u, v)$ as the amount of additional flow allowed without exceeding $c(u, v)$, given by

$$c_f(u, v) = c(u, v) - f(u, v) \quad (4.2)$$

Given a flow network $G = (V, E)$, its corresponding residual network $G_f = (V, E_f)$ with respect to a flow f consists of the same vertices in V but has a different set of edges, E_f . The edges in the residual network, called the *residual edges*, are weighted edges, whose weights are the residual capacities of the corresponding edges in E . The weights of residual edges should always be positive. For every pair of vertices in E , there exist up to two residual edges connecting them with opposite directions in G_f . Figure 4.20 shows the residual network G_f of the flow network G in Figure 4.19. Notice that, for the vertex pair v_1 and v_3 in G , there are two residual edges in G_f , (v_1, v_3) and (v_3, v_1) . We see that $c_f(v_3, v_1) = 2$, because we can push a flow with a value of two in G to cancel out its original flow. On the other hand, there should be three residual edges between v_2 and v_3 in G_f , one from v_2 to v_3 and two from v_3 to v_2 . However, the residual edges of the same direction will be merged as one edge only. Therefore, $c_f(v_3, v_2) = 7 + 6 = 13$.

We can easily find augmenting paths in the residual network, because they are just simple paths from the source to the sink. The amount of additional flow that can be pushed into an augmenting path p is determined by the residual capacity of p , $c_f(p)$, which is defined as the minimum residual capacity of all edges on the path. For example, $s \rightarrow v_2 \rightarrow v_3 \rightarrow t$ is an augmenting path p in Figure 4.20. Its residual capacity $c_f(p) = 2$ is determined by the residual edge (v_3, t) . Therefore, we can push extra flow with a value of two through p in the original flow network. By repeatedly finding augmenting paths in the

**FIGURE 4.20**

The residual network G_f of the flow network G in Figure 4.19 in which the augmenting path is shown by the thickened lines.

residual network and updating the residual network, a maximum-flow problem can be solved. The next Subsection shows two algorithms implementing this idea.

4.3.8.3 The Ford-Fulkerson method and the Edmonds-Karp algorithm

The *Ford-Fulkerson method* is a classical means of finding maximum flows [Ford 1962]. It simply finds augmenting paths on the residual network until no more paths exist. The pseudocode is presented in Algorithm 4.15.

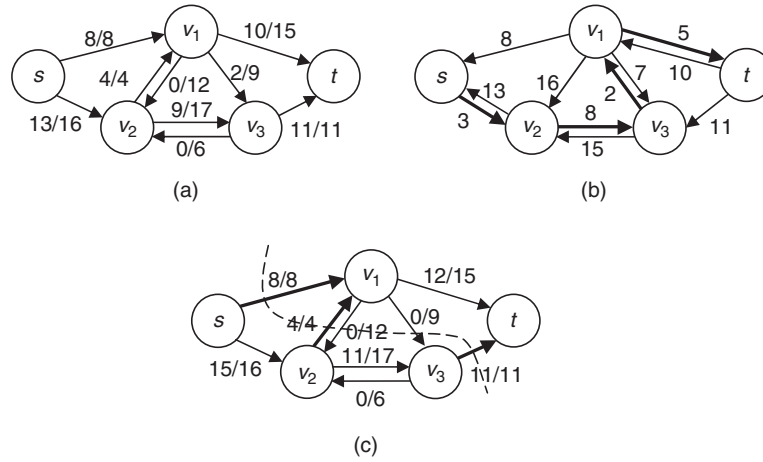
Algorithm 4.15 Ford-Fulkerson method

Ford-Fulkerson(Graph G , Source s , Sink t)

1. **for** (each $(u, v) \in E$) $f[u, v] = f[v, u] = 0$;
 2. Build a residual network G_f based on flow f ;
 3. **while** (there is an augmenting path p in G_f) **do**
 4. $c_f(p) = \min(c_f(u, v) : (u, v) \in p)$;
 5. **for** (each edge $(u, v) \in p$) **do**
 6. $f[u, v] = f[u, v] + c_f(p)$;
 7. $f[v, u] = -f[u, v]$;
 8. **end for**
 9. Rebuild G_f based on new flow f ;
 10. **end while**
-

We can apply the Ford-Fulkerson method to the flow network G in Figure 4.19. Figure 4.21a shows the result of adding the augmenting path to G in Figure 4.20. The function `Ford-Fulkerson` gives us the result in Figure 4.21c. The maximum flow, denoted as f^* , has a value of 23.

We call this the *Ford-Fulkerson method* rather than *algorithm*, because the approach to finding augmenting paths in a residual graph is not fully specified. This ambiguity costs precious runtime. The Ford-Fulkerson method has a time complexity of $O(E \cdot |f^*|)$. It takes $O(E)$ time to construct a residual network and each augmenting path increases the flow by at least 1. Therefore, we build the residual

**FIGURE 4.21**

(a) Adding the augmenting path found in Figure 4.20 to G of Figure 4.19. (b) The resultant residual network of (a) with an augmenting path p . (c) Adding p to (a) results in a maximum flow of value 23. The dashed line is the minimum cut with a value of 23.

networks at most $|f^*|$ times. $|f^*|$ is not an input parameter for the maximum-flow problem, so the Ford-Fulkerson method does not have a polynomial-time complexity. It will be a serious problem if $|f^*|$ is as great as, say, 1,000,000,000.

The ambiguity present in the Ford-Fulkerson method is fixed by the *Edmonds-Karp algorithm* [Edmonds 1972]. Instead of blindly searching for any augmenting paths, the Edmonds-Karp algorithm uses *breadth-first search* to find the augmenting path with a minimum number of edges in the residual network. For an edge in the residual work, there can be many augmenting paths passing through it in different iterations. It can be proven that for every edge in the residual network, the lengths of the augmenting paths passing through it will only increase with the advancement of iterations [Ahuja 1993; Cormen 2001]. Because the upper limit of the length of an augmenting path is $|V| - 1$, there exist $O(V)$ different augmenting paths passing through a specific edge. Therefore, there exist $O(VE)$ different augmenting paths and thus $O(VE)$ constructions of residual networks, resulting in a time complexity of $O(E \cdot VE) = O(VE^2)$.

4.3.8.4 Cuts and the max-flow min-cut theorem

Until now we have not proven the correctness of finding the maximum flow by use of residual networks. In this subsection, we introduce an important concept in the flow network—*cuts*. The *max-flow min-cut theorem* is used to prove the correctness of the Ford-Fulkerson method and the Edmonds-Karp algorithm.

A *cut* (S, T) of the flow network $G = (V, E)$ is a partition of V that divides V into two subsets, S and $T = V - S$, such that the source $s \in S$ and the sink $t \in T$. The *net flow* across the cut (S, T) is denoted as $f(S, T)$:

$$f(S, T) = \sum_{u \in S, v \in T} f(u, v) \quad (4.3)$$

The *capacity* of the cut (S, T) , $c(S, T)$, is defined as

$$c(S, T) = \sum_{u \in S, v \in T} c(u, v) \quad (4.4)$$

Notice that only those edges incident from S to T are counted according to (4.4). Take Figure 4.21a as an example. For the cut $(\{s, v_2, v_3\}, \{v_1, t\})$, its net flow is:

$$f(s, v_1) + f(v_2, v_1) + f(v_3, v_1) + f(v_3, t) = 8 + 4 + (-2) + 11 = 21$$

and its capacity is:

$$c(s, v_1) + c(v_2, v_1) + c(v_3, t) = 8 + 4 + 11 = 23$$

We can observe that for any cut (S, T) , the property $f(S, T) \leq c(S, T)$ always holds. The number of possible cuts in a flow network grows exponentially with the number of vertices. We are particularly interested in finding a **minimum cut**, which is the cut with a minimum capacity among all possible cuts in a network.

With the knowledge of cuts in a flow network, we can explain the max-flow min-cut theorem. For a flow f in a flow network $G = (V, E)$, the **max-flow min-cut theorem** states that the following three conditions are equivalent:

- (1) f is a maximum flow in G .
- (2) The residual network G_f has no augmenting paths.
- (3) $|f| = c(S, T)$ for some cut of G .

We first prove (1) \Rightarrow (2). If f is a maximum flow in G and there is still an augmenting path p in G_f , then the sum of flow $|f| + c_f(p) > |f|$, which is a contradiction. Secondly, we prove (2) \Rightarrow (3). Suppose G_f has no augmenting path or, equivalently, there is no path in G_f from s to t . We define $S = \{v \in V \text{ such that } v \text{ is reachable from } s \text{ in } G_f\}$ and $T = V - S$. The partition (S, T) is a cut. For any edge (u, v) across the cut, we have $f(u, v) = c(u, v)$ because $(u, v) \notin G_f$, so $f(S, T) = c(S, T)$. It can be reasoned that $|f| = f(S, T)$ as follows:

$$|f| = f(s, V) = f(s, V) + f(S - s, V) = f(S, V) = f(S, V) - f(S, S) = f(S, T)$$

with $f(S - s, V) = 0$, because the source s is excluded. As a result, we can see that $|f| = f(S, T) = c(S, T)$. Finally, we prove (3) \Rightarrow (1) by use of the property $|f| \leq c(S, T)$ of any cut (S, T) . Because $f(u, v) \leq c(u, v)$ for any edge across the cut (S, T) , $|f| = f(S, T) \leq c(S, T)$. And if a flow f^* has $|f^*| = c(S^*, T^*) \geq |f|$ for a specific cut (S^*, T^*) , then the flow f^* must be a maximum flow and the cut (S^*, T^*) must be a minimum cut.

The **max-flow min-cut theorem** not only proves that finding augmenting paths in a residual network is a correct way to solve the maximum-flow problem, it also proves that finding a maximum flow is equivalent to finding a

minimum cut. In Figure 4.21c, we see that the maximum flow found indeed has the same value as the cut $(\{s, v_2, v_3\}, \{v_1, t\})$.

Finding a minimum cut has many EDA applications, such as dividing a module into two parts with a minimum interconnecting wire length. We can thus solve this kind of problem with a maximum-flow algorithm.

4.3.8.5 Multiple sources and sinks and maximum bipartite matching

In some applications of the maximum-flow problem, there can be more than one source and more than one sink in the flow network. For example, if we want to count the number of paths from a set of inputs to a set of outputs in an electrical circuit, there would be multiple sources and multiple sinks. However, we can still model those flow networks as a single-source, single-sink network by use of a *supersource* and a *supersink*. Given a flow network with sources s_i , $1 \leq i \leq m$ and sinks t_j , $1 \leq j \leq n$, a supersource s connects the sources with edges (s, s_i) and capacities $c(s, s_i) = \infty$. Similarly, a supersink t is created with edges (t_j, t) and capacities $c(t_j, t) = \infty$. With this simple transformation, a flow network with multiple sources and sinks can be solved with common maximum-flow algorithms.

Maximum bipartite matching is an important application of the multiple-source, multiple-sink maximum flow problem. A *bipartite graph* $G = (V, E)$ is an undirected graph whose vertices are partitioned into two sets, L and R . For each edge $(u, v) \in E$; if $u \in L$, then $v \in R$, and vice versa. Figure 4.22a gives an example of a bipartite graph. A *matching* on an undirected graph $G = (V, E)$ is a subset of edges $M \subseteq E$ such that for all $v \in V$, at most one edge of M is incident on v . *Maximum matching* is a matching that contains a maximum number of edges. The *maximum bipartite matching* problem is the problem of finding a maximum matching on a bipartite graph. Figure 4.22a shows such a maximum matching with three edges on a bipartite graph.

The maximum bipartite graph problem itself has many useful applications in the field of EDA. For example, technology mapping can be modeled as a

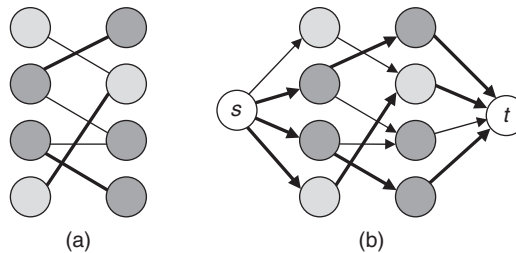


FIGURE 4.22

(a) A bipartite graph with its maximum matching indicated by thickened lines. (b) The corresponding flow network provides the solution to the maximum bipartite matching problem. Every edge has unit capacity.

bipartite graph. The functional modules to be mapped are modeled as vertices on one side, and all cell libraries of the target technology are vertices on the other side. We can solve the maximum bipartite graph problem by solving the corresponding multiple-source, multiple-sink maximum graph problem as shown in Figure 4.22b. The Ford-Fulkerson method can solve this problem with a time complexity of $O(VE)$ because $|f^*| \leq |V|/2$.

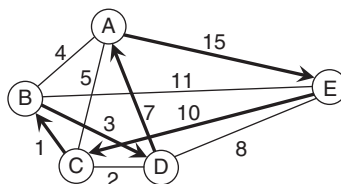
4.4 HEURISTIC ALGORITHMS

Heuristic algorithms are algorithms that apply heuristics, or rules of thumb, to find a good, but not necessarily optimal, solution for the target problem. The heuristics in such algorithms function as guidelines for selecting good solutions from possible ones. Notice that good solutions, rather than optimal solutions, are found in heuristic algorithms, which is the biggest difference between heuristics and other types of algorithms. To compensate for this disadvantage, heuristic algorithms generally have much lower time complexity. For problems that are either large in size or computationally difficult (NP-complete or NP-hard, or both) other types of algorithms may find the best solutions but would require hours, days, or even years to identify such a solution. Heuristic algorithms are the preferred method for these types of problems because they sacrifice some solution quality while saving a huge amount of computational time.

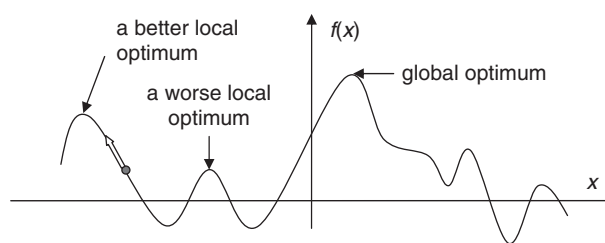
NP-complete and NP-hard problems are currently prevalent in the EDA applications. For example, the Traveling Salesman Problem (TSP, see Section 4.2) has many EDA applications such as routing, but TSP optimization is an NP-hard problem. In a TSP problem with n cities (nodes), a brute-force search for the shortest route results in an overwhelmingly high time complexity of $O(n!)$. For these sorts of problems, heuristic algorithms are often a better and necessary choice.

Heuristic algorithms empirically yield good, and sometimes optimal, solutions. The solution quality, however, cannot be guaranteed. For example, there is a greedy algorithm (see Subsection 4.4.1 for more details) called the Nearest Neighbor (NN) algorithm that can be used to solve the TSP problem. NN lets the salesman start from any one city and then travel to the nearest unvisited city at each step. NN quickly generates a short route with a $O(n^2)$ time complexity, given n as the number of cities. Nevertheless, there are some examples showing that this intuitive algorithm yields inefficient routes. In Figure 4.23, applying NN and starting from city C results in the route $C \rightarrow B \rightarrow D \rightarrow A \rightarrow E \rightarrow C$ whose total length is $1 + 3 + 7 + 15 + 10 = 36$; however, traversing the cities in the loop $C \rightarrow D \rightarrow E \rightarrow A \rightarrow B \rightarrow C$ is a shorter route: $2 + 8 + 15 + 4 + 1 = 31$. This example shows that we have to be cautious when we use heuristic algorithms, because they can sometimes yield poor solutions.

In this section, we discuss several frequently used heuristic algorithms. *Greedy algorithms*, *dynamic programming*, and *branch-and-bound* algorithms are heuristic algorithms that direct the search toward a solution space

**FIGURE 4.23**

An inefficient route yielded by the Nearest Neighbor algorithm.

**FIGURE 4.24**

Local versus global optima for a one-dimensional function. From a current solution (gray dot), greedy algorithms try to make a greedy choice that bring it toward a local optimum, which may be different from a global optimal one.

that promises a better solution quality. *Simulated annealing* and *genetic algorithms* exert a series of perturbations on current solutions, trying to ameliorate them through the process. These heuristic algorithms have extensive EDA applications [Reeves 1993].

4.4.1 Greedy algorithm

Algorithms targeting an optimization problem typically consist of a series of stages with choices made at each of these stages. A *greedy algorithm*, which aims to solve an optimization problem, makes choices at every stage toward a local optimum and with the hope of eventually reaching a globally optimal solution. Greedy algorithms get their name from the fact that these algorithms always make a choice that looks like the best possible solution at the moment without thoroughly considering the underlying conditions and consequences that may result from that choice, acting much like a greedy person. Figure 4.24 illustrates the difference between local and global optima for a one-dimensional function.

In fact, we often exploit the concept of greedy algorithms in our daily lives without knowing it. For instance, making change in sequence by use of the minimum number of coins is a typical situation illustrating this concept. Suppose we want to give change of 36 cents in U.S. currency. The coins that can be used consist of the 25-cent quarter, the 10-cent dime, the 5-cent nickel, and the

1-cent penny. Then, we apply a rule of thumb: pick the coin of the greatest value that is less than the change amount first. The change will consequently be made in this sequence: a quarter (25 cents), a dime (10 cents), and a penny (1 cent)—a total of three coins. This rule of thumb leads to the minimum number of coins, three, because it perfectly embodies the essence of greedy algorithms: making greedy choices at each moment. In this particular problem, a greedy algorithm yields the optimal solution.

However, greedy algorithms do not always produce optimal solutions. Let us revisit the making change example. If a coin with a value of 20 cents exists, the rule of thumb just mentioned would not lead to the minimum number of coins if the amount of change needed was 40 cents. By applying the rule of picking the coin of highest value first, we would be giving change of a quarter (25 cents), a dime (10 cents) and a nickel (5 cents), a total of three coins, but, in fact, two, 20-cent coins would be the optimal solution for this example. The greedy algorithm fails to reach the optimal solution for this case.

Actually, the example given previously is not ideal for illustrating the concept of greedy algorithms, because it violates the *optimal substructure* property. In general, problems suitable for greedy algorithms must exhibit two characteristics: the *greedy-choice* property and the *optimal substructure* property. If we can demonstrate that a problem has these two properties, then a greedy algorithm would be a good choice.

4.4.1.1 Greedy-choice property

The **greedy-choice property** states that a globally optimal solution can always be achieved by making locally optimal, or greedy, choices. By locally optimal choices we mean making choices that look best for solving the current problem without considering the results from other subproblems or the effect(s) that this choice might have on future choices.

In Section 4.4, we introduced the Nearest Neighbor (NN) algorithm for solving—more precisely, for approximating—an optimal solution to TSP. NN is a greedy algorithm that picks the nearest city at each step. NN violates the greedy-choice property and thus results in suboptimal solutions, as indicated in the example of Figure 4.23. In Figure 4.23, the choice of $B \rightarrow D$ is a greedy one, because the other remaining cities are further from B. In a globally optimal solution, the route of either $D \rightarrow C \rightarrow B$ or $B \rightarrow C \rightarrow D$ is a necessity, and the choice of $B \rightarrow D$ is suboptimal. Hence, NN is not an optimal greedy algorithm, because TSP does not satisfy the greedy-choice property.

Making change with a minimum number of coins is an interesting example. On the basis of the current U.S. coins, this problem satisfies the greedy-choice property. But when a 20-cent coin comes into existence, the property is violated—when making change for 40 cents, the greedy choice of picking a quarter affects the solution quality of the rest of the problem.

How do we tell if a particular problem has the greedy-choice property? In a greedy algorithm designed for a particular problem, if any greedy choice can be

proven better than all of the other available choices at the moment in terms of solution quality, we can say that the problem exhibits the greedy-choice property.

4.4.1.2 *Optimal substructure*

A problem shows **optimal substructure** if a globally optimal solution to it consists of optimal solutions to its subproblems. If a globally optimal solution can be partitioned into a set of subsolutions, optimal substructure requires that those subsolutions must be optimal with respect to their corresponding subproblems. Consider the previous example of making change of 36 cents with a minimum number of coins. The optimal solution of a quarter, a dime, and a penny can be divided into two parts: (1) a quarter and a penny and (2) a dime. The first part is, indeed, optimal in making change of 26 cents, as is the second part for making change of 10 cents.

The NN algorithm for TSP lacks both greedy-choice and optimal substructure properties. Its global solutions cannot be divided into solutions for its subproblems, let alone optimal solutions.

To determine whether a particular problem has an optimal substructure, two aspects have to be examined: *substructure* and *optimality*. A problem has substructure if it is divisible into subproblems. *Optimality* is the property that the combination of optimal solutions to subproblems is a globally optimal solution.

Greedy algorithms are highly efficient for problems satisfying these two properties. On top of that, greedy algorithms are often intuitively simple and easy to implement. Therefore, greedy algorithms are very popular for solving optimization problems. Many graph algorithms, mentioned in Section 4.3, are actually applications of greedy algorithms—such as Prim’s algorithm used for finding minimum spanning trees. Greedy algorithms often help find a lower bound of the solution quality for many challenging real-world problems.

4.4.2 Dynamic programming

Dynamic programming (DP) is an algorithmic method of solving optimization problems. *Programming* in this context refers to mathematical programming, which is a synonym for optimization.

DP solves a problem by combining the solutions to its subproblems. The famous divide-and-conquer method also solves a problem in a similar manner. The divide-and-conquer method divides a problem into independent subproblems, whereas in DP, either the subproblems depend on the solution sets of other subproblems or the subproblems appear repeatedly. DP uses the dependency of the subproblems and attempts to solve a subproblem only once; it then stores its solution in a table for future lookups. This strategy spares the time spent on recalculating solutions to old subproblems, resulting in an efficient algorithm.

To illustrate the superiority of DP, we show how to efficiently multiply a chain of matrices by use of DP. When multiplying a chain of matrices, the order of the multiplications dramatically affects the number of scalar multiplications. For example,

consider multiplying three matrices A, B, and C whose dimensions are 30×100 , 100×2 , and 2×50 , respectively. There are two ways to start the multiplication: either $A \cdot B$ or $B \cdot C$ first. The numbers of necessary scalar multiplications are:

$$\begin{aligned} (A \cdot B) \cdot C &: 30 \times 100 \times 2 + 30 \times 2 \times 50 = 6000 + 3000 = 9000, \\ A \cdot (B \cdot C) &: 100 \times 2 \times 50 + 30 \times 100 \times 50 = 10,000 + 150,000 = 160,000 \end{aligned}$$

$(A \cdot B) \cdot C$ is clearly more computationally efficient.

The **matrix-chain multiplication problem** can be formulated as follows: given a chain of n matrices, $\langle M_1, M_2, \dots, M_n \rangle$, where M_i is a $v_{i-1} \times v_i$ matrix for $i = 1$ to n , we want to find an order of multiplication that minimizes the number of scalar multiplications.

To solve this problem, one option is to exhaustively try all possible multiplication orders and then select the best one. However, the number of possible multiplication orders grows exponentially with respect to the number of matrices n . There are only two possibilities for three matrices, but it increases to 1,767,263,190 possibilities for 20 matrices. A brute-force search might cost more time finding the best order of multiplications than actually performing the multiplication.

Here, we define $m[i, j]$ as the minimum number of scalar multiplications needed to calculate the matrix chain $M_i M_{i+1} \dots M_j$, for $1 \leq i \leq j \leq n$. The target problem then becomes finding $m[1, n]$. Because a matrix chain can be divided into two smaller matrix chains, each of which can be multiplied into a single matrix first, the following recurrent relationship holds:

$$m[i, j] = \begin{cases} 0 & \text{if } i = j \\ \min_{i \leq k < j} \{m[i, k] + m[k + 1, j] + v_{i-1} v_k v_j\} & \text{if } i < j \end{cases} \quad (4.5)$$

A simple recursive algorithm on the basis of recurrence (4.5) can provide the answer to $m[1, n]$; however, such an algorithm will be extremely inefficient because, in the process of computing $m[1, n]$, many entries of $m[i, j]$ are computed multiple times. For example, if we wish to compute $m[1, 6]$, the value of $m[3, 4]$ will be repeatedly computed in the process of calculating $m[1, 4]$, $m[2, 5]$, and $m[3, 6]$. However, we could store the values in a table, which leads to the dynamic programming algorithm `BottomUpMatrixChain` shown in Algorithm 4.16.

Algorithm 4.16 A dynamic programming algorithm for solving the matrix-chain multiplication problem

`BottomUpMatrixChain(Vector v)`

1. $n = v.size - 1$;
2. **for** ($i = 1$ to n) $m[i, i] = 0$;
3. **for** ($p = 2$ to n) **do** // p is the chain length


```

4.  for ( $i = 1$  to  $n - p + 1$ ) do
5.     $j = i + p - 1$ ;
6.     $m[i, j] = \infty$ ;
7.    for ( $k = i$  to  $j - 1$ ) do
8.       $temp = m[i, k] + m[k + 1, j] + v_{i-1}v_kv_j$ ;
9.      if ( $temp < m[i, j]$ ) do
10.         $m[i, j] = temp$ ;
11.         $d[i, j] = k$ ;
12.      end if
13.    end for
14.  end for
15. return  $m$  and  $d$ ;

```

The `BottomUpMatrixChain` perfectly embodies the property of recurrence (4.5). A triangular table $m[i, j]$, where $1 \leq i \leq j \leq n$, records the minimum numbers of scalar multiplications for its respective matrix chains, whereas another triangular table $d[i, j]$, where $1 \leq i < j \leq n$, tracks where the separations of matrix chains should be. We can see in line 3 that the m table is filled in the ascending order of the length of the matrix chains, so that in line 8, the items to be added are already in place. Finally, the fully filled m and d tables are returned as answers in line 15.

`BottomUpMatrixChain` handles recurrence (4.5) by making use of the repetitive nature of the subproblems. The three loops in lines 3, 4, and 7 indicate that this algorithm has a time complexity of $O(n^3)$. Compared with the exponential time needed to search through all possible multiplication orders, `BottomUpMatrixChain` is highly efficient.

`BottomUpMatrixChain` is a typical example of dynamic programming. It solves the matrix-chain multiplication problem by systematically combining solutions to multiplication of smaller matrix chains. In fact, the matrix-chain multiplication problem contains two key ingredients that make `BottomUpMatrixChain` a successful function: *overlapping subproblems* and *optimal substructure*. These two properties are indispensable for any DP algorithm to work.

4.4.2.1 Overlapping subproblems

We say that a problem has *overlapping subproblems* when it can be decomposed into subproblems that are not independent of one another. Often several subproblems share the same smaller subproblems. For example, running a recursive algorithm often requires solving the same subproblem multiple times. DP solves each subproblem only once and stores the answer in a table, so that

recurrences of the same subproblems take only constant time to get the answer (by means of a table lookup).

The matrix-chain multiplication problem is an instance of this property. Repeated multiplications of smaller matrix chains cause a high complexity for a simple recursive algorithm. In contrast, the DP algorithm `BottomUpMatrixChain` creates the m table for the overlapping subproblems to achieve high efficiency.

4.4.2.2 Optimal substructure

A problem exhibits an **optimal substructure** if its globally optimal solution consists of optimal solutions to the subproblems within it. Recall that in Subsection 4.4.1, having an optimal substructure ensures that greedy algorithms yield optimal solutions. In fact, if a problem has an optimal substructure, both greedy algorithms and DP could yield optimal solutions. One key consideration in choosing the type of algorithm is determining whether the problem has the greedy-choice property, the overlapping subproblems, or neither. If the problem shows overlapping subproblems but not the greedy-choice property, DP is a better way to solve it. On the other hand, if the problem exhibits the greedy-choice property instead of overlapping subproblems, then a greedy algorithm fits better. A problem rarely has both of the properties because they contradict each other. The matrix-chain multiplication problem has an optimal substructure, reflected in recurrence (4.4), but it does not have the greedy-choice property. It consists of overlapping subproblems. Therefore, DP is a suitable approach to address this problem.

4.4.2.3 Memoization

`BottomUpMatrixChain`, as its name suggests, solves the problem iteratively by constructing a table in a bottom-up fashion. A top-down approach, on the other hand, seems infeasible, from this simple recursive algorithm. In fact, the unnecessary recomputations that prevent the recursive algorithm from being efficient can be avoided by recording all the computed solutions along the way. This idea of constructing a table in a top-down recursive fashion is called **memoization**. The pseudocode of a *memoized* DP algorithm to solve the matrix-chain multiplication problem is shown in Algorithm 4.17.

Algorithm 4.17 Solving matrix-chain multiplication problems with memoization

`TopDownMatrixChain(Vector v)`

1. $n = v.size - 1$;
2. **for** ($i = 1$ to n)
3. **for** ($j = i$ to n) $m[i, j] = \infty$;
4. **return** Memoize($v, 1, n$);

`Memoize(Vector v, Index i, Index j)`

1. **if** ($m[i, j] < \infty$) **return** $m[i, j]$;

```

2. if ( $i = j$ )  $m[i, j] = 0$ ;
3. else
4.   for ( $k = i$  to  $j - 1$ ) do
5.      $temp = \text{Memoize}(v, i, k) + \text{Memoize}(v, k + 1, j) + v_{i-1}v_kv_j$ ;
6.     if ( $temp < m[i, j]$ )  $m[i, j] = temp$ ;
7.   end for
8. end if
9. return  $m[i, j]$ ;

```

The time complexity of the `TopDownMatrixChain` shown in Algorithm 4.17 is still $O(n^3)$, because it maintains the m table. The actual runtime of the `TopDownMatrixChain` will be slightly longer than the `BottomUpMatrixChain` because of the overhead introduced by recursion. In general, memorization can outperform a bottom-up approach only if some subproblems need not be visited. If every subproblem has to be solved at least once, the bottom-up approach should be slightly better.

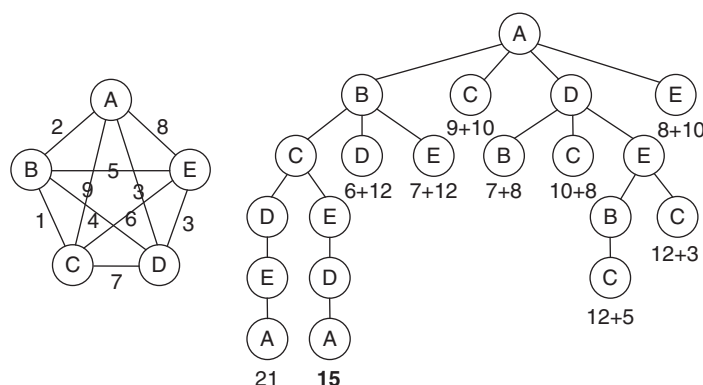
4.4.3 Branch-and-bound

Branch-and-bound is a general technique for improving the searching process by systematically enumerating all candidate solutions and disposing of obviously impossible solutions.

Branch-and-bound usually applies to those problems that have finite solutions, in which the solutions can be represented as a sequence of options. The first part of branch-and-bound, **branching**, requires several choices to be made so that the choices *branch out* into the solution space. In these methods, the solution space is organized as a treelike structure. Figure 4.25 shows an instance of TSP and a solution tree, which is constructed by making choices on the next cities to visit.

Branching out to all possible choices guarantees that no potential solutions will be left uncovered. But because the target problem is usually NP-complete or even NP-hard, the solution space is often too vast to traverse. The branch-and-bound algorithm handles this problem by **bounding** and **pruning**. Bounding refers to setting a bound on the solution quality (*e.g.*, the route length for TSP), and pruning means trimming off branches in the solution tree whose solution quality is estimated to be poor. Bounding and pruning are the essential concepts of the branch-and-bound technique, because they are used to effectively reduce the search space. We demonstrate in Figure 4.25 how branch-and-bound works for the TSP problem.

The number under a leaf node of the solution tree represents the length of the corresponding route. For incomplete branches, an expression in the form of $a + b$ is shown. In this notation, a is the length of the traversed edges, and

**FIGURE 4.25**

A TSP and its solution tree after applying branch-and-bound.

b is a lower bound for the length of the remaining route that has not been explored. The lower bound is derived by use of a *minimum spanning tree* that consists of the unvisited vertices, as well as the root and leaf vertices of the partial route. For example, for the unfinished route $A \rightarrow B \rightarrow E$, a minimum spanning tree is built for nodes A, C, D, and E, and its value is 12. This lower bound is a true underestimate for the length of the remaining route. The sum of these two numbers provides the basis for bounding.

The solution tree is traversed depth-first, with the length of the current shortest route as the upper bound for future solutions. For example, after $A \rightarrow B \rightarrow C \rightarrow D \rightarrow E \rightarrow A$ is examined, the upper bound is 21, and after the next route is explored, the bound drops to 15. Every time a partial route is extended by a vertex, a lower bound for the length of the rest of the route is computed. If the sum $a + b$ is over or equal to the current upper bound, the solutions on that branch guarantees to be worse than the current best solution, and the branch can be pruned. Most branches are pruned in Figure 4.25.

An exhaustive search will build a search tree with 89 nodes,¹ but the solution tree with branch-and-bound has only 20 nodes. Branch-and-bound accelerates the search process by reducing the solution space *en masse*. Although branch-and-bound algorithms generally do not possess proven time complexity, their efficiency has made them the first choice for many problems, especially for NP-complete problems.

Branch-and-bound mainly addresses optimization problems, because bounding is often based on numerical comparisons. TSP that uses the route length as the bound is a classical application; however, it can also be applied to some decision problems. In these cases, the bounding criteria are often restrictions or

¹Let n be the number of cities and $f(n)$ be the number of nodes in the exhausted search tree. Then $f(2) = 3$, $f(3) = 7$, and $f(n) = (n-1)f(n-1) + 1$.

additional descriptions of possible solutions. The **Davis-Putnam-Logemann-Loveland (DPLL)** search scheme for the Boolean Satisfiability problem is a typical and important application for this kind of branch-and-bound algorithm.

4.4.4 Simulated annealing

Simulated annealing (SA) is a general probabilistic algorithm for optimization problems [Wong 1988]. It uses a process searching for a global optimal solution in the solution space analogous to the physical process of *annealing*. In the process of annealing, which refines a piece of material by heating and controlled cooling, the molecules of the material at first absorb a huge amount of energy from heating, which allows them to wander freely. Then, the slow cooling process gradually deprives them of their energy, but grants them the opportunity to reach a crystalline configuration that is more stable than the material's original form. The idea to use simulated annealing on optimization problems was first proposed by S. Kirkpatrick, C. D. Gelatt, and M. P. Vecchi in [Kirkpatrick 1983] for the placement and global routing problems.

Simulated annealing (SA) is analogous to annealing in three ways:

1. The energy in annealing corresponds to the **cost function** in SA. The cost function evaluates every solution, and the cost of the best-known solution generally decreases during the SA process. The goal of an optimization problem is to find a solution with a minimum cost.
2. The movements of molecules correspond to small **perturbations** in the current solution, such as switching the order of two consecutive vertices in a solution to TSP. SA repeatedly perturbs the current solution so that different regions in the solution space are explored.
3. The temperature corresponds to a control parameter **temperature T** in SA. T controls the probability of accepting a new solution that is worse than the current solution. If T is high, the acceptance probability is also high, and *vice versa*. T starts at the peak temperature, making the current solution changes almost randomly at first. T then gradually decreases, so that more and more suboptimal perturbations are rejected. The algorithm normally terminates when T reaches a user-specified value.

An SA algorithm typically contains two loops, an outer one and an inner one. In the outer loop, T dwindles every time, and the outer loop terminates when T reaches some user-specified value. In the inner loop, the solution is perturbed, and the cost function of the perturbed solution is evaluated. If the new solution has a lower cost, it directly replaces the current solution. Otherwise, to accept or reject the new, higher-cost solution is based on a probability function that is positively related to T and negatively related to the cost difference between the current and new solutions. The inner loop continues until a *thermal equilibrium* is reached, which means that T also controls the number of iterations

of the inner loop. After both loops terminate, the best solution visited in the process is returned as the result.

The pseudocode in Algorithm 4.18 outlines the SA algorithm. There are a few details worth discussion: in line 2 of the function `Accept`, the number $e^{-\frac{\Delta c}{T}}$ ensures that a higher cost solution has a greater likelihood of acceptance if T is high or the cost difference (Δc) is small. Although there is no strong theoretical justification for the need of strictly following this exact formula, this formula has been popular among SA users.

Algorithm 4.18 Simulated annealing algorithm

`Accept(temperature T , cost Δc)`

1. Choose a random number *rand* between 0 and 1;
2. **return** ($e^{-\Delta c/T} > \text{rand}$);

`SimulatedAnnealing()`

1. solution *sNow*, *sNext*, *sBest*;
 2. temperature T , *endingT*;
 3. Initialize *sNow*, T and *endingT*;
 4. **while** ($T > \text{endingT}$) **do**
 5. **while** (!`ThermalEquilibrium(T)`)**do**
 6. *sNext* = `Perturb(sNow)`;
 7. **if** (`cost(sNext) < cost(sNow)`)
 8. *sNow* = *sNext*;
 9. **if** (`cost(sNow) < cost(sBest)`)
 10. *sBest* = *sNow*;
 11. **else if** (`Accept(T, cost(sNext)-cost(sNow))`)
 12. *sNow* = *sNext*;
 13. **end if**
 14. **end while**
 15. Decrease(T);
 16. **end while**
 17. **return** *sBest*;
-

The combination of the functions `ThermalEquilibrium`, `Decrease`, and the parameter *endingT* in Algorithm 4.18 characterize an SA algorithm. In combination, they determine the *cooling schedule* or the *annealing schedule*. The cooling schedule can be tuned in many ways, such as making T drop faster at first and slower afterwards in the function `Decrease` or allowing more perturbations when T is small in the function `ThermalEquilibrium`. Every

adjustment in the cooling schedule affects the solution quality and the time taken to find a solution. In practice, empirical principles and a trial-and-error strategy are commonly used to find a good cooling schedule [Hajek 1988].

SA has many advantages over other optimization algorithms. First, because there is a non-zero probability of accepting higher cost solutions in the search process, SA avoids becoming stuck at some local minima, unlike some greedy approaches. Also, the runtime of SA is controllable through the cooling schedule. One can even abruptly terminate this algorithm by changing the parameter *endingT* in line 4 of *SimulatedAnnealing*. Finally, there is always a best-known solution available no matter how little time has elapsed in the search process. With SA, the user can always get a solution. In general, a longer runtime would result in a better-quality solution. This flexibility explains SA's wide popularity. SA is considered the top choice for several EDA problems, such as placement and Binary Decision Diagram (BDD) variable reordering.

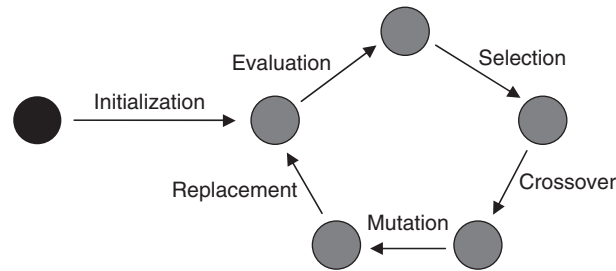
4.4.5 Genetic algorithms

Just like simulated annealing, *genetic algorithms* are another general randomized algorithm catering to optimization problems [Goldberg, 1989; Davis 1991]. They also perform a series of computations to search for a global optimal solution in the solution space. As the name suggests, genetic algorithms use techniques inspired by operations found in evolutionary biology such as selection, crossover, and mutation.

Genetic algorithms are different from other global search heuristics in many ways. First of all, other global search algorithms, such as simulated annealing, perform a series of perturbations on a single solution to approach a global optimum. Genetic algorithms simultaneously operate on a set of feasible solutions or a *population*. Moreover, the solutions in a genetic algorithm are always encoded into strings of mathematical symbols, which facilitate future manipulations on them. Many types of coding symbols can be used, such as bits, integers, or even permutations. In the simplest versions of genetic algorithms, fixed-length bit strings are used to represent solutions. A bit string that specifies a feasible solution is called a *chromosome*. Each bit in a chromosome is called a *gene*.

Genetic algorithms have many variations [Holland 1992]. Here we will focus on the *simple genetic algorithm* (SGA) to get a taste of the mechanics of genetic algorithms. SGA can be separated into six phases: initialization, evaluation, selection, crossover, mutation, and replacement. After the initial population is generated in the **initialization** phase, the other five actions take place in turns until termination. Figure 4.26 shows the flow of SGA.

In the **evaluation** phase, chromosomes in the population are evaluated with a *fitness function*, which indicates how good the corresponding solutions are. Their *fitness values* are the criteria of selection in the next phase. Advanced

**FIGURE 4.26**

The flow of a simple genetic algorithm.

genetic algorithms can even handle multi-purposed optimization problems with plural fitness functions.

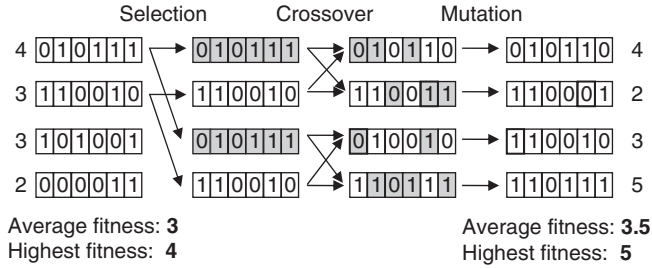
The **selection** phase aims at finding the best parents or a group of solutions to generate the next population. Many schemes can be implemented to exercise selection in SGA. The simplest scheme is *truncation selection*, in which the s chromosomes with the highest fitness values are chosen, and l/s copies are duplicated for each of them, in which l is the population size. Notice that the population size will not change after selection. Another simple selection scheme, Roulette-Wheel selection, chooses a chromosome with the probability of the ratio of its fitness value to the sum of all fitness values of the population.

In the **crossover** phase, children chromosomes are produced by inheriting genes from pairs of parent chromosomes. As always, there are many methods to implement the crossover, each with its pros and cons. *Uniform crossover* states that every gene of a child chromosome comes from a dad with a probability of p (usually 0.5) and from a mom with a probability of $(1 - p)$. Conventionally, two parents give birth to two children so that the population size remains unchanged.

Mutation means changing a tiny fraction of the genes in the chromosomes. Although in biology mutations rarely happen, they do prevent genetic algorithms from getting stuck in local minima. After the processes of evaluation, selection, crossover, and mutation are complete, the new population **replaces** the old one and the next iteration begins.

Figure 4.27 shows a tiny example of an SGA, with a population size of four and chromosome length of six. The fitness function simply counts “1” genes. *Truncation selection* and *uniform crossover* with a probability of 0.5 are used in this example. Notice that the average and highest fitness values increase after one generation.

In this example, the best solution seems very easy to achieve, so an SGA seems unnecessary; however, in real-life applications of SGA, a population size can be as large as 100,000 and a chromosome can contain up to 10,000 genes. The fitness function will be much more complex as well.

**FIGURE 4.27**

One-generation simulation of a simple genetic algorithm.

SGA is just a small part of the broad subject of genetic algorithms. Genetic algorithms remain an active research topic for various applications. In addition to EDA, they have applications in a variety of fields, including designing shapes for high-speed trains and human face recognition.

4.5 MATHEMATICAL PROGRAMMING

Mathematical programming, or mathematical optimization, is a systematic approach used for optimizing (minimizing or maximizing) the value of an objective function with respect to a set of constraints. The problem in general can be expressed as:

$$\begin{aligned} &\text{Minimize (or maximize) } f(x); \\ &\text{Subject to } X = \{X | g_i(x) \leq b_i, i = 1 \dots m\} \end{aligned}$$

where

- $x = (x_1, \dots, x_n)$ are optimization (or decision) variables,
- $f : R^n \rightarrow R$ is the objective function, and
- $g_i : R^n \rightarrow R$ and $b_i \in R$ form the constraints for the valid values of x

4.5.1 Categories of mathematical programming problems

According to the natures of f and X , mathematical programming problems can be classified into several different categories:

1. If $X = R^n$, the problem is unconstrained;
2. If f and all the constraints are linear, the problem is called a *linear programming* (LP) problem. The linear constraints can then be represented in the matrix form:

$$Ax \leq b$$

where A is an $m \times n$ matrix corresponding to the coefficients in $g_i(x)$.

3. If the problem is linear, and all the variables are constrained to integers, the problem is called an *integer linear programming* (ILP) problem. If only some of the variables are integers, it is called a *mixed integer linear programming* (MILP or MIP) problem.
4. If the constraints are linear, but the objective function f contains some quadratic terms, the problem is called a *quadratic programming* (QP) problem.
5. If f or any of $g_i(x)$ is not linear, it is called a *nonlinear programming* (NLP) problem.
6. If all the constraints have the following convexity property:

$$g_i(\alpha x_a + \beta x_b) \leq \alpha g_i(x_a) + \beta g_i(x_b)$$

where $\alpha \geq 0$, $\beta \geq 0$, and $\alpha + \beta = 1$, then the problem is called a *convex programming* or *convex optimization* problem.

7. If the set of feasible solutions defined by f and X are discrete, the problem is called a *discrete* or *combinatorial optimization* problem.

Intuitively speaking, different categories of mathematical programming problems should involve different solving techniques, and, thus, they may have different computational complexities. In fact, most of the mathematical optimization problems are generally intractable—algorithms to solve the preceding optimization problems such as the *Newton method*, *steepest gradient*, *branch-and-bound*, etc., often require an exponential runtime or an excessive amount of memory to find the *global* optimal solutions. As an alternative, people turn to heuristic techniques such as *hill climbing*, *simulated annealing*, *genetic algorithms*, and *tabu search* for a reasonably good local optimal solution.

Nevertheless, some categories of mathematical optimization problems, such as linear programming and convex optimization, can be solved efficiently and reliably. Therefore, it is feasible to examine whether the original optimization problem can be modeled or approximated as one of these problems. Once the modeling is completed, the rest should be easy—there are numerous shareware or commercial tools available to solve these standard problems.

In the following, we will briefly describe the problem definitions and solving techniques of the linear programming and convex optimization problems. For more theoretical details, please refer to other textbooks or lecture notes on this subject.

4.5.2 Linear programming (LP) problem

Many optimization problems can be modeled or approximated by linear forms. Intuitively, solving LP problems should be simpler than solving the general mathematical optimization problems, because they only deal with linear constraint and objective functions; however, it took people several decades to

develop a polynomial time algorithm for LP problems, and several related theoretical problems still remain open [Smale 2000].

The *simplex algorithm*, developed by George Dantzig in 1947, is the first practical procedure used to solve the LP problem. Given a set of n -variable linear constraints, the simplex algorithm first finds a basic feasible solution that satisfies all the constraints. This basic solution is conceptually a *vertex* (i.e., an *extreme point*) of the convex polyhedron expanded by the linear constraints in R^n hyperspace. The algorithm then moves along the *edges* of the polyhedron in the direction toward finding a better value of the objective function. It is guaranteed that the procedure will eventually terminate at the optimal solution.

Although the simplex algorithm can be efficiently used in most practical applications, its worst-case complexity is still exponential. Whether a polynomial time algorithm for LP problems exists remained unknown until the late 1970s, when Leonid Khachiyan applied the ellipsoid method to this problem and proved that it can be solved in $O(n^4w)$ time. Here n and w are the number and width of variables, respectively.

Khachiyan's method had theoretical importance, because it was the first polynomial-time algorithm that could be applied to LP problems; however, it did not perform any better than the simplex algorithm for most practical cases. Many researchers who followed Khachiyan focused on improving the average case performance, as well as the computational worst-case complexity. The most noteworthy improvements included Narendra Karmarkar's interior point method and many other revised simplex algorithms [Karmarkar 1984].

4.5.3 Integer linear programming (ILP) problem

Many of the linear programming applications are concerned with variables only in the integral domain. For example, signal values in a digital circuit are under a modular number system. Therefore, it is very likely that optimization problems defined with respect to signals in a circuit can be modeled as ILP problems. On the other hand, problems that need to enumerate the possible cases, or are related to scheduling of certain events, are also often described as ILP.

The ILP problem is in general much more difficult than is LP. It can be shown that ILP is actually one of the NP-hard problems. Although the formal proof of the computational complexity of the ILP problem is beyond the scope of this book, we will use the following example to illustrate the procedure and explain the difficulty in solving the ILP problem.

The ILP problem in Figure 4.28 is to maximize an objective function f , with respect to four linear constraints $\{g_1, g_2, g_3, g_4\}$. Because the problem consists of only two variables, x and y , it can be illustrated on a two-dimensional plane, where each constraint is a straight line, the four constraints form a closed region C , and the feasible solutions are the lattice or integral points within this region. The objective function f , represented as a straight line to the right of region C , moves in parallel with respect to different values of k . Intuitively, to obtain

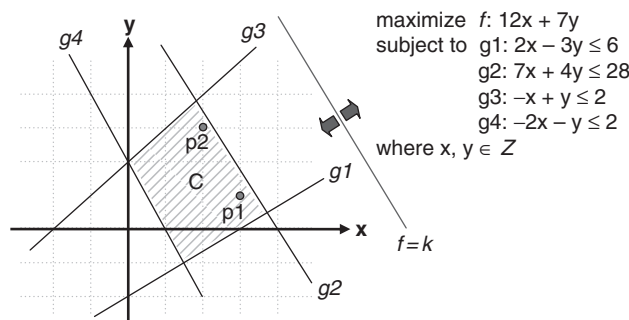


FIGURE 4.28

An ILP example.

the maximum value of f , we can move the line $f = k$ from where it is located in the figure until it intersects the region C on a lattice point for the first time.

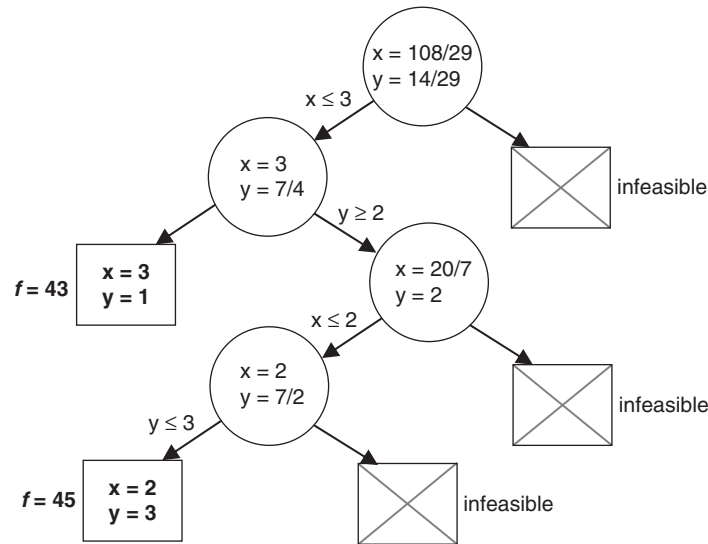
From the figure, it is clear that the maximum value must occur on either point p_1 (3, 1) or p_2 (2, 3). For p_1 , $f = 12 \times 3 + 7 \times 1 = 43$, and for p_2 , $f = 12 \times 2 + 7 \times 3 = 45$. Therefore, the maximum value of f is 45, which occurs at $(x, y) = (2, 3)$.

This solving procedure is not applicable for ILP problems with more variables—it will be impossible to visualize the constraints and to identify the candidate integral points for the optimum solutions. In fact, to find a feasible assignment that satisfies all the constraints of an ILP problem is already an NP-complete problem. Finding an optimal solution is even more difficult.

4.5.3.1 Linear programming relaxation and branch-and-bound procedure

Because it is very difficult to directly find a feasible solution that satisfies all the constraints of the ILP problem, one popular approach is to relax the integral constraints on the variables and use a polynomial-time linear programming solver to find an approximated nonintegral solution first. Then, on the basis of the approximated solution, we can apply a branch-and-bound algorithm to further narrow the search [Wolsey 1998].

In the previous example, the LP relaxation tells us that the optimal solution occurs at $(x, y) = (108/29, 14/29)$. Because x is an integer, we can branch on variable x into two conditions: $x \leq 3$ and $x \geq 4$. For $x \geq 4$, the LP solver will report infeasibility because the union of the constraints is an empty set. On the other hand, for the $x \leq 3$ case we will have the optimal solution at $(x, y) = (3, 7/4)$. Because y is not yet an integer, we further branch on y — $y \leq 1$ and $y \geq 2$. For $y \leq 1$, we obtain an integral solution $(x, y) = (3, 1)$ and $f = 43$. For $y \geq 2$, the LP optimal solution will be $(x, y) = (20/7, 2)$. Repeating the above process, we will eventually acquire the integral optimal solution

**FIGURE 4.29**

Decision tree of the LP-based branch-and-bound.

$(x, y) = (2, 3)$ and $f = 45$. The decision graph of the branch-and-bound process is shown in Figure 4.29.

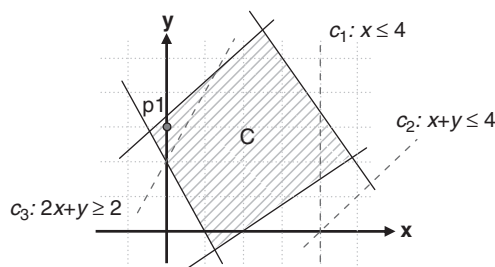
4.5.3.2 Cutting plane algorithm

Another useful approach for solving ILP problems is the cutting plane algorithm. This algorithm iteratively adds valid inequalities to the original problem to narrow the search area enclosed by the constraints while retaining the feasible points. Figure 4.30 illustrates an example of such valid inequalities.

In Figure 4.30, the cuts c_1 and c_2 are said to be *valid inequalities*, because all the feasible points (*i.e.*, the integral points within the dash region C) are still valid after adding the new constraints. On the other hand, cut c_3 is not a valid inequality because one feasible point p_1 becomes invalid afterward.

It is clear to see that the addition of the valid inequality c_2 will not help the search for the optimal solution because it does not narrow the search region. On the contrary, cut c_1 is said to be a *strong* valid inequality because it makes the formulation “stronger.” The goal of the cutting plane algorithm is to add such strong valid inequalities in the hope that the optimal solution will eventually become an extreme point of the polyhedron so that it can be found by the polynomial-time LP algorithm.

There are many procedures to generate valid inequalities such as *Chvátal-Gomory* [Gomory 1960], *0-1 Knapsack* [Wolsey 1999], and *lift-and-project* [Balas 1993] *cuts*. However, sheer use of these valid inequality generation procedures in the cutting plane algorithm will not go too far in solving difficult ILP

**FIGURE 4.30**

Valid and invalid inequalities.

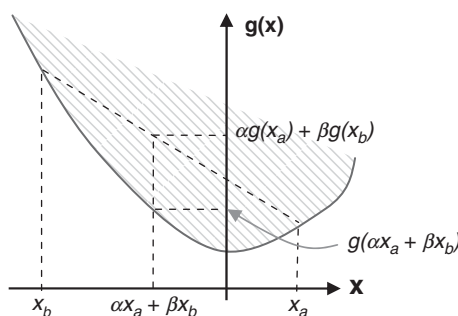
problems—it may take an exponential number of steps to approach an integral extreme point. A better approach would be combining the cutting plane algorithm with the branch-and-bound process. This combined technique is called the branch-and-cut algorithm.

4.5.4 Convex optimization problem

As mentioned in Subsection 4.5.1, the constraints in the convex optimization problem are convex functions with the following convexity property (Figure 4.31):

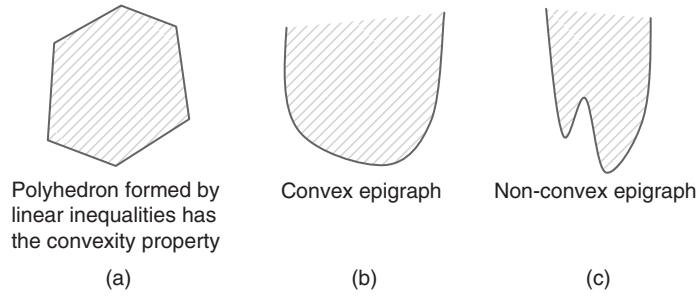
$$g_i(\alpha x_a + \beta x_b) \leq \alpha g_i(x_a) + \beta g_i(x_b)$$

where $\alpha \geq 0$, $\beta \geq 0$, and $\alpha + \beta = 1$. Conceptually, the convexity property can be illustrated as follows:

**FIGURE 4.31**

The convexity property.

In other words, given two points x_a and x_b from the set of points defined by a convex function, all the points on the line segment between x_a and x_b will also belong to the set (*i.e.*, the dash region), which is called a *convex set*. Moreover, it can be shown that for a convex function, a local optimal solution is also a global optimal solution. In addition, the intersection of multiple convex sets is also convex [Boyd 2004].

**FIGURE 4.32**

Examples of convex functions.

More examples of convex functions can be found in Figure 4.32. The LP problem, where its constraints form a polyhedron in the n -dimensional hyperspace, is a special case of the convex optimization problem.

4.5.4.1 Interior-point method

Similar to linear programming, there is, in general, no analytical formula for the solution of a convex optimization problem. However, there are many effective methods that can solve the problems in polynomial time within a reasonably small number of iterations. The *interior-point* method is one of the most successful approaches.

Although detailed comprehension of the interior-point method requires the introduction of many mathematical terms and theorems, we can get a high-level view of the method by comparing it with the simplex method as shown in Figure 4.33. In the simplex method, we first obtain an initial feasible solution and then refine it along the edge of the polyhedron until the optimal solution is reached. In the interior-point method, the initial feasible solution is approximated as an interior point. Then, the method iterates along a path, called a *central path*, as the approximation improves toward the optimal solution.

One popular way to bring the interior-point solution to the optimal one is by the use of a *barrier function*. The basic idea is to rewrite the original problem into an *equality formula* so that Newton's method can be applied to find the optimal solution.²

Let's first define an *indicator function* $I(u)$ such that $I(u) = 0$ if $u \leq 0$, and $I(u) = \infty$ otherwise (Figure 4.34). We can then combine the convex objective function $\min f(x)$, and the constraints $g_i(x) \leq 0 \mid i = 1 \sim m$ as:

$$\min \left(f(x) + \sum_{i=1}^m I(g_i(x)) \right)$$

²To apply the Newton's method, the formula needs to be an equality and twice differentiable.

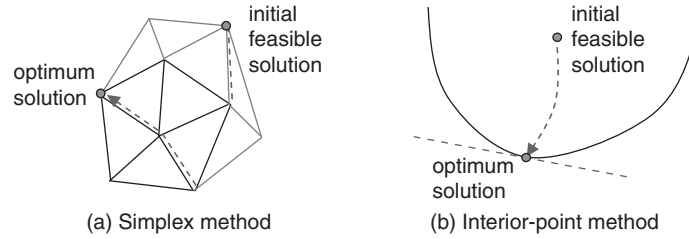


FIGURE 4.33

Comparison of simplex and interior-point methods.

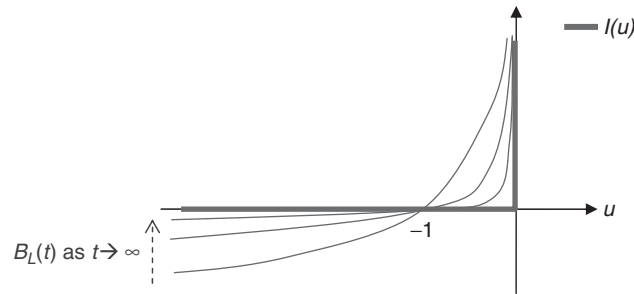


FIGURE 4.34

Indicator $I(u)$ and logarithmic functions B_L .

This formula describes the same problem as the original convex optimization problem and after the rewrite, there are no more inequalities. However, this formula is not twice differentiable (*i.e.*, not *smooth*) near $u = 0$, so Newton's method cannot work. One solution is to use the following *logarithmic barrier function* to approximate the indicator function:

$$B_L(u, t) = -(1/t)\log(-u)$$

where $t > 0$ is a parameter to control the approximation. As t approaches infinity, the logarithmic barrier function $B_L(u)$ gets closer to the indicator function $I(u)$.

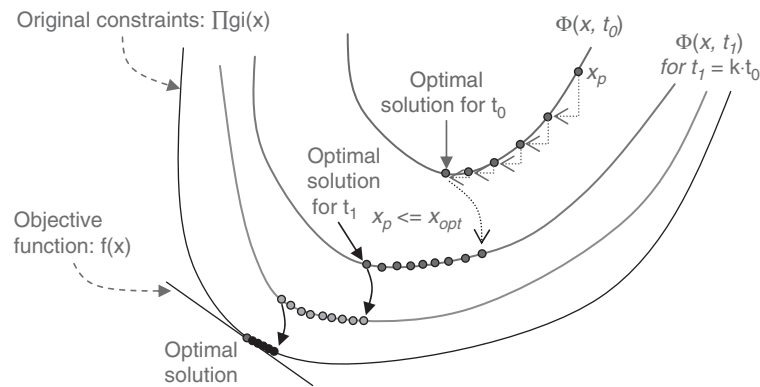
By use of the logarithmic barrier function, the objective function then becomes:

$$\min \left(f(x) + \sum_{i=1}^m -(1/t)\log(-g_i(x)) \right)$$

Please note that now the optimization formula is convex and twice differentiable (we assume that both $f(x)$ and $g_i(x)$ are twice differentiable here). Therefore, we can apply Newton's method iteratively and eventually reach an optimal

InteriorMethod (objFunction f, Constraints g)

1. Let $(x, t) = \min(f(x) + \sum_1^m - (1/t)\log(-g_i(x)))$
2. Given initial t , tolerance ϵ
3. Find an interior feasible point x_p s.t. $\forall i, g_i(x_p) < 0$
4. Starting from x_p , apply Newton's method to find the optimal solution x_{opt}
5. If $(\frac{1}{t} < \epsilon)$ return optimality as $\{x_{opt}, (x_{opt}, t)\}$;
6. Let $x_p = x_{opt}$, $t = k \cdot t$ for $k > 1$, repeat 4

**FIGURE 4.35**

Interior-point algorithm and an illustration of its concept.

solution. However, please remember that this will be just an approximate solution because of the introduction of the logarithmic barrier function.

The questions then arise: How close is this solution to the solution of the original problem? What is the effect of t ? Intuitively, if t gets larger, the final solution will be closer to the solution of the original convex optimization problem. However, with a larger t , it will take a longer time for Newton's method to converge. On the other hand, the use of a smaller t will lead to a faster solution at the cost of accuracy.

The pseudocode in Figure 4.35 is an interior-point algorithm that gives a solution balancing runtime and accuracy. We first start with a smaller t so that Newton's method converges faster. Once the optimal solution for this t value is obtained, we then increase t so that the optimal solution gradually approaches the real optimization of the original problem. This process terminates when the inverse of the variable t becomes less than the specified tolerance ϵ .

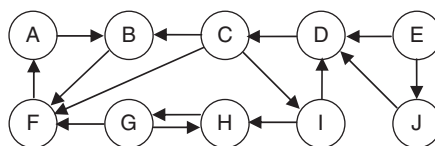
4.6 CONCLUDING REMARKS

In this chapter, we present various fundamental algorithms to the EDA research and development—from the classic graphic theories, the practical heuristic approaches, and then to the theoretical mathematical programming techniques. The readers are advised to get acquainted with these algorithms to completely appreciate the spirit of the research in different areas of the later chapters.

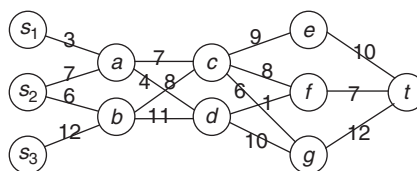
In addition, please note that a good EDA algorithm is usually *hybrid*. In other words, it should act as a *strategy*, or say *problem-solving tactic* that is able to apply different algorithms in different situations. It should be working efficiently for the most common cases, taking advantage of the easy ones, and at the same time, handling the worst-case scenarios gracefully. In summary, do not just take the algorithms in this chapter as ready solutions; instead, thoroughly understand the problems first, consider the trade-offs between runtime and memory, and then treat the algorithms as different utilities, or weapons, for the different challenges in the EDA problem solving process.

4.7 EXERCISES

- 4.1. **(Computational Complexity)** Rank the following functions by order of growth by use of asymptotic notations. One function is neither $O(f_i)$ nor $\Omega(f_i)$ for any other functions f_i . Which is that?
 - a. $4^{\lg n}$
 - b. $n \cdot 2^n$
 - c. $n^n \cdot \cos n$
 - d. $n \cdot \lg n$
 - e. $(n + 1)!$ f. $\lg^{999} n$ g. $n \cdot \lg n$ h. $n^{1/\lg n}$
- 4.2. **(Computational Complexity)** A *Hamiltonian path* in a graph is a simple path that visits every vertex exactly once. The decision problem HAMILTONIAN PATH for a graph G and vertices u and v asks whether a Hamiltonian path exists from u to v in G .
 - a. Prove that HAMILTONIAN PATH is NP.
 - b. Given that HAMILTONIAN PATH is NP-complete, prove that HAMILTONIAN CYCLE is also NP-complete.
- 4.3. **(Graph Algorithms)** Figure 4.36 shows a directed graph of 10 vertices. How many strongly connected components does this graph have and which are they?
- 4.4. **(Graph Algorithms)** Given an undirected, weighted graph $G = (V, E)$ and two vertices u and v in V . Find an efficient path from u to v such that the biggest edge weight on the path is minimized.

**FIGURE 4.36**

A directed graph to find strongly connected components.

**FIGURE 4.37**

A model for a combinational circuit in which vertices represent gates and edge weights stand for the number of connecting wires, where gates s_1 , s_2 , and s_3 have to be in one module and t in the other, and meanwhile minimizing the number of wires crossing two modules. What is the minimal number of crossing wires and where should the cut of two modules be?

- 4.5. (Graph Algorithms)** The weighted, undirected graph illustrated in Figure 4.37 models a combinational circuit. We want to divide these gates (vertices) into two modules.
- 4.6. (Heuristic Algorithms)** In a dance class, n male students and n female students should be paired. If we want to minimize the sum of height differences of the n pairs,
- Design a *greedy algorithm* to efficiently solve this problem.
 - Prove that the algorithm works because the problem exhibits both the greedy-choice and optimal substructure properties.
- 4.7. (Heuristic Algorithms)** Solve the matrix-chain multiplication problem if the dimensions of the matrices are 5×10 , 10×3 , 3×12 , 12×5 , 5×50 , and 50×6 . What are the minimum number of scalar multiplications needed and the order of the multiplications?
- 4.8. (Heuristic Algorithms)** Use the *branch-and-bound* technique to solve the TSP problem in Figure 4.38. What is the length of the shortest route? If only the branching technique is used to form the search tree, what is the number of tree nodes?
- 4.9. (Linear Programming)** Given an $n \times m$ rectangular, which is composed of equal-length (length = 1) matches as shown in Figure 4.39.
- In this problem, we will try to remove as few as possible matches so that all the squares (including 1×1 , 2×2 , 3×3 , ...) in the

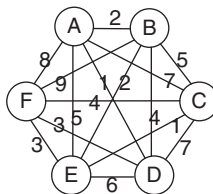


FIGURE 4.38

A TSP instance.

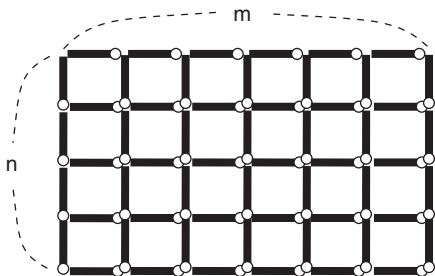


FIGURE 4.39

A square-breaking problem.

rectangular are broken. Please model this problem as an integer linear programming (ILP) problem.

4.10. (Convex Optimization) Prove that a local optimum of a convex function must be a global optimum.

ACKNOWLEDGMENTS

We thank Dr. Bow-Yaw Wang of Academia Sinica, Taiwan, and Mr. Benjamin Liang of University of California, Berkeley, for their thorough reviews of the entire chapter, and Professor Tian-Li Yu of National Taiwan University for providing valuable comments on the “Genetic Algorithm” subsection.

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