# Chapter 2

# Classic Discrete Optimization Problems

Often, an excellent way to begin work on a project involving modeling is to look at an informal representation of the problem we need to solve and ask whether it reminds us of any problem we have seen before. We may have to simplify the problem a bit or distort aspects of it to match it to something we already know how to solve. Nonetheless, this can be a good way to get a first pass at a solution. Later on, we can look at whether the problem can be modified to restore important aspects of the real system that were removed in that first pass. The same basic algorithm can often accommodate fairly large changes in the model.

The purpose of this chapter is to help with this process by examining some of the classic discrete optimization problems that we are likely to see reflected in applied work. I have tried to focus here on problems that might "look hard" if we are not familiar with them, since those are the problems for which it is most valuable to know what is and is not doable. For readers who have taken an introductory algorithms class, this chapter will be largely a review, but hopefully a useful one. Some of these problems already have important applications in practical computational biology. Others come up often enough in other applied contexts that we might consider them good guesses when looking for solutions to new problems. When looking at a modeling problem for which we do not yet have a solution, we can try to run through some of the problems in this chapter and see if any of them remind us of the problem we need to solve.

We will begin by looking at graph problems. Graphs have proven to be a very useful abstraction for a broad range of optimization problems in computational biology. We will then consider some important string and sequence problems. These two abstractions are broadly important to computer science in general, although particularly so to computational biology. We will then examine some of the issues in adapting classic algorithms to a real-world problems through a minicase study on the topic of building intraspecies phylogenies (evolutionary trees).

#### 2.1 Graph Problems

We will start with a quick review of graphs. A graph G consists of a set of nodes, V, and a set of edges, E. Each edge  $e_i$  is defined by a pair of nodes  $(v_i, v_j)$ . A graph can be directed, meaning  $(v_i, v_j) \neq (v_i, v_i)$ , or undirected, meaning  $(v_i, v_j) = (v_j, v_i)$ . It can also be weighted, meaning

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#### **Table of Contents Optimization Problems Stu Schwartz**

- 1. Understanding the eBook Optimization Problems Stu Schwartz
  - The Rise of Digital Reading Optimization Problems Stu Schwartz
  - Advantages of eBooks Over Traditional Books
- 2. Identifying Optimization Problems Stu Schwartz
  - Exploring Different Genres
  - Considering Fiction vs. Non-Fiction
  - Determining Your Reading Goals
- 3. Choosing the Right eBook Platform
  - Popular eBook Platforms
  - Features to Look for in an Optimization Problems Stu Schwartz
  - User-Friendly Interface
- 4. Exploring eBook Recommendations from Optimization Problems Stu Schwartz
  - Personalized Recommendations
  - o Optimization Problems Stu Schwartz User Reviews and Ratings
  - Optimization Problems Stu Schwartz and Bestseller Lists
- 5. Accessing Optimization Problems Stu Schwartz Free and Paid eBooks
  - o Optimization Problems Stu Schwartz Public Domain eBooks
  - o Optimization Problems Stu Schwartz eBook Subscription Services
  - Optimization Problems Stu Schwartz Budget-Friendly Options
- 6. Navigating Optimization Problems Stu Schwartz eBook Formats
  - o ePub, PDF, MOBI, and More
  - o Optimization Problems Stu Schwartz Compatibility with Devices
  - Optimization Problems Stu Schwartz Enhanced eBook Features
- 7. Enhancing Your Reading Experience
  - Adjustable Fonts and Text Sizes of Optimization Problems Stu Schwartz
  - Highlighting and Note-Taking Optimization Problems Stu Schwartz
  - Interactive Elements Optimization Problems Stu Schwartz
- 8. Staying Engaged with Optimization Problems Stu Schwartz

- Joining Online Reading Communities
- Participating in Virtual Book Clubs
- Following Authors and Publishers Optimization Problems Stu Schwartz
- 9. Balancing eBooks and Physical Books Optimization Problems Stu Schwartz
  - Benefits of a Digital Library
  - Creating a Diverse Reading Collection Optimization Problems Stu Schwartz
- 10. Overcoming Reading Challenges
  - Dealing with Digital Eye Strain
  - Minimizing Distractions
  - Managing Screen Time
- 11. Cultivating a Reading Routine Optimization Problems Stu Schwartz
  - Setting Reading Goals Optimization Problems Stu Schwartz
  - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Optimization Problems Stu Schwartz
  - Fact-Checking eBook Content of Optimization Problems Stu Schwartz
  - Distinguishing Credible Sources
- 13. Promoting Lifelong Learning
  - Utilizing eBooks for Skill Development
  - Exploring Educational eBooks
- 14. Embracing eBook Trends
  - o Integration of Multimedia Elements
  - Interactive and Gamified eBooks

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