

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 mini case 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 $(v_i, v_j) \neq (v_j, v_i)$, or undirected, meaning $(v_i, v_j) = (v_j, v_i)$. It can also be weighted, meaning

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