

# APPROXIMATION ALGORITHMS FOR THE FIXED-TOPOLOGY PHYLOGENETIC NUMBER PROBLEM\*

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**Abstract.** In the  $\ell$ -phylogeny problem, one wishes to construct an evolutionary tree for a set of species represented by characters, in which each state of each character induces no more than  $\ell$  connected components. We consider the fixed-topology version of this problem for fixed-topologies of arbitrary degree. This version of the problem is known to be  $\mathcal{NP}$ -complete for  $\ell \geq 3$  even for degree-3 trees in which no state labels more than  $\ell + 1$  leaves (and therefore there is a trivial  $\ell + 1$  phylogeny). We give a 2-approximation algorithm for all  $\ell \geq 3$  for arbitrary input topologies and we give an optimal approximation algorithm that constructs a 4-phylogeny when a 3-phylogeny exists. Dynamic programming techniques, which are typically used in fixed-topology problems, cannot be applied to  $\ell$ -phylogeny problems. Our 2-approximation algorithm is the first application of linear programming to approximation algorithms for phylogeny problems. We extend our results to a related problem in which characters are polymorphic.

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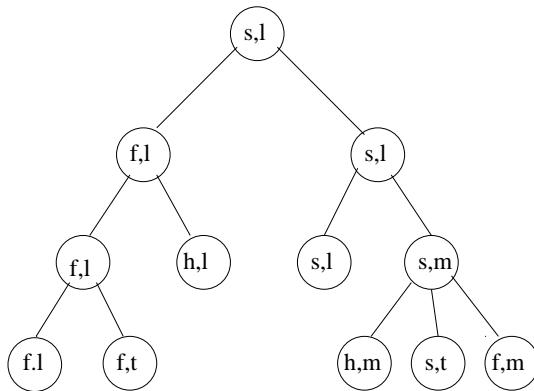


FIG. 1. An example of a 2-phylogeny. States  $h$  and  $f$  in the first character and state  $t$  in the second character are each in two components.

**1. Introduction.** The evolutionary biologist collects information on extant species (and fossil evidence) and attempts to infer the evolutionary history of a set of species. Most mathematical models of this process assume divergent evolution, meaning that once two species diverge, they never share genetic material again. Therefore, evolution is modelled as a tree (*phylogeny*), with extant species as leaves and (extant, extinct, or hypothesized) ancestors as internal nodes. Species have been modelled in several ways, depending upon the nature of available information and the mechanism for gathering that information. Based upon these representations, differing measures of evolutionary distance and objective function are used to evaluate the goodness of a proposed evolutionary tree.

In this paper we assume that input data is character-based. Let  $S$  be an input set of  $n$  species. A *character*  $c$  is a function from the species set  $S$  to a set  $R_c$  of **states**. The set of species in figure 1 has two characters. The first character represents skin covering and has three states:  $h$  for hair,  $s$  for scales, and  $f$  for feathers. The second character represents size, where  $t$  (tiny) means at most one foot long,  $m$  (medium) means one to three feet long and  $l$  (large) means greater than three feet long. If we are given a set of characters  $c_1, \dots, c_k$  for  $S$ , each species is a vector from  $R_{c_1} \times \dots \times R_{c_k}$  and any such vector can represent a hypothesized ancestor. For example, an anaconda (the largest known species of snake) would be represented on these simple characters as  $(s, l)$  and a hummingbird would be  $(f, t)$ . Characters can be used to model biomolecular data, such as a column in a multiple sequence alignment, but in this paper, we think of characters as morphological properties such as coloration or the ability to fly.

Character-based phylogenies are typically evaluated by some *parsimony-like* measure, meaning that the total evolutionary change is somehow minimized. In this paper, we consider the  $\ell$ -*phylogeny* metric introduced in [9]. Given a phylogenetic tree, a character  $c_i$  and a state  $j \in R_{c_i}$ , let  $\ell_{ij}$  be the number of connected components in  $c_i^{-1}(j)$  (the subtree induced by the species with state  $j$  in character  $i$ ). A phylogeny is an  $\ell$ -*phylogeny* if each state of each character induces no more than  $\ell$  connected components. That is,  $\max_{c_i, j \in R_{c_i}} \ell_{ij} \leq \ell$ . The  $\ell$ -*phylogeny problem* is to determine if an input consisting of a species set  $S$  and a set of characters  $c_1, \dots, c_k$  has an  $\ell$ -*phylogeny*. The *phylogenetic number* problem is to determine the minimum  $\ell$  such that the input has an  $\ell$ -*phylogeny*.

The classic parsimony problem is to find a tree that minimizes the total number

of evolutionary changes:  $\sum_{c_i, j \in R_{c_i}} \ell_{ij}$ . The compatibility problem is to maximize the number of characters that are *perfect*, meaning that all states of that character induce only one connected component. Thus the compatibility problem is to maximize  $|\{c_i : \ell_{ij} = 1 \text{ for all } j \in R_{c_i}\}|$ . A 1-phylogeny is called a *perfect phylogeny*. All three problems ( $\ell$ -phylogeny for  $\ell \geq 1$ , parsimony, compatibility) are  $\mathcal{NP}$ -complete [1, 9, 4, 5, 6, 8, 14]. Papers [4, 5, 8] prove that different restrictions of the classic parsimony problem are  $\mathcal{NP}$ -complete<sup>1</sup>. Parsimony,  $\ell$ -phylogeny, and compatibility all allow states of a character to evolve multiple times. However, both parsimony and compatibility allow some characters to evolve many times. The  $\ell$ -phylogeny metric requires *balanced* evolution, in that no one character can pay for most of the evolutionary changes. Thus,  $\ell$ -phylogeny is a better measure than parsimony or compatibility in biological situations in which all characters are believed to evolve slowly.

In this paper we consider the *fixed-topology* variant of the  $\ell$ -phylogeny problem, where in addition to the species set and characters, we are also given a tree  $T$  in which internal nodes are unlabelled, each leaf is labelled with a species  $s \in S$  and each species  $s \in S$  is the label of exactly one leaf of  $T$ . The *fixed-topology  $\ell$ -phylogeny problem* is the problem of determining labels for the internal nodes so that the resulting phylogeny is an  $\ell$ -phylogeny, or determining that such a labelling does not exist. In figure 1, the hypothesized ancestor  $(s, m)$  labels one node. This example is a 2-phylogeny.

Fixed-topology algorithms can be used as *filters*. Current phylogeny-producing software can generate thousands of trees which are (approximately) equally good under some metric such as maximum likelihood or parsimony. We can think of these outputs as proposed topologies. One way to differentiate these hypotheses is to see which topologies also have low phylogenetic number. For example, the original trees can be generated by biomolecular sequence data, and they can then be filtered using morphological data with slowly-evolving traits.

It will be convenient to allow a node to remain unlabelled in one or more characters in a fixed topology. In this case, the node disagrees with all of its neighbors on all unlabelled characters. We can easily extend such a labelling to one in which every node is labelled without increasing  $\ell_{ij}$  for any  $i$  or  $j$ : for any character  $j$ , for each connected component of nodes which are not labelled, choose any neighbouring node  $v$  which is labelled  $i_v$  and label the entire component with the state  $i_v$ . This does not introduce any extra component for  $i_v$ , nor does it break components of any other state that weren't already broken.

In the fixed-topology setting, optimal trees for the parsimony and compatibility metrics can be found in polynomial time [7]. The fixed-topology  $\ell$ -phylogeny problem can be solved in polynomial time for  $\ell \leq 2$ , but is  $\mathcal{NP}$ -complete for  $\ell \geq 3$  even for degree-3 trees in which no state labels more than  $\ell + 1$  leaves (and therefore there is a trivial  $\ell + 1$  phylogeny) [9]. Fitch's algorithm for parsimony uses dynamic programming. Dynamic programming also gives good algorithms in some cases for finding phylogenies when characters are polymorphic [2].

Jiang, Lawler, and Wang [11] consider the fixed-topology tree-alignment problem, where species are represented as biomolecular sequences, the cost of an edge in the tree is the edit distance between the labels at its endpoints, and the goal is to minimize the sum of the costs over all edges. They give a 2-approximation for bounded-degree

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<sup>1</sup> Wareham[17] describes and corrects a minor error in the reduction used by Day in [4] to show the  $\mathcal{NP}$ -completeness of the problem for Wagner characters.

input topologies and extend this to obtain a polynomial-time approximation scheme (PTAS). In Lemma 3 of [11], they prove that the best lifted tree (in which the label of each internal node is equal to the label of one of its children) is within a factor of 2 of the best tree with arbitrary labels. The proof only uses the triangle inequality (it does not use any other facts about the cost measure). Therefore, the result holds for several other cost measures, including  $\ell$ -phylogeny, parsimony, and the minimum-load cost measure for phylogenies with polymorphic characters which was introduced in [2]. It also holds for the variant of  $\ell$ -phylogeny in which  $\ell_i$  is specified for each character  $c_i$ . This variant was introduced in [9]. We refer to it as the *generalized  $\ell$ -phylogeny problem*. In fact, Lemma 3 of [11] holds for the fixed-topology problem with *arbitrary* input topologies, though the authors do not state this fact since they do not use it. Despite the applicability of Lemma 3, the algorithmic method of Jiang, Lawler and Wang does not seem to be useful in developing approximation algorithms for the fixed-topology  $\ell$ -phylogeny problem (or for related problems). Jiang et al. use dynamic programming to find the minimum-cost lifted tree. Dynamic programming is not efficient for the more global metric of  $\ell$ -phylogeny. The dynamic programming proceeds by computing an optimal labelling for a subtree for each possible labelling of the root of the subtree. For metrics where cost is summed over edges (such as parsimony or tree alignment), one only needs to find the lowest-cost labelling for a given root label. For the  $\ell$ -phylogeny problem, the cost of a tree depends upon how many times each state is broken for a given character. One cannot tell *a priori* which state will be the limiting one. Therefore, instead of maintaining a single optimal tree for each root label, we must maintain all trees whose cost (represented as a vector of components for each state) is undominated. This number can be exponential in  $r$ , the number of states, even for bounded-degree input trees. This is a common theme in combinatorial optimization: the more global nature of minimax makes it harder to compute than summation objectives, but also more useful.

Gusfield and Wang [15] take the approach of [11] a step further by proving that the best uniform lifted tree (ULT) is within a factor of 2 of the best arbitrarily-labelled tree. In a uniform lifted tree on each level, all internal nodes are labeled by the same child (e.g. all nodes at level one take the label of their leftmost child). This proof also extends to the  $\ell$ -phylogeny metric. If the input tree is a complete binary tree, then there are only  $n$  ULTs, and exhaustive search is efficient, giving an algorithm which is faster than ours and has an equivalent performance bound. However, when the input tree isn't complete (even if it is binary), Gusfield and Wang use dynamic programming to find the minimum-cost ULT, and so their method fails when it is applied to the  $\ell$ -phylogeny problem. Wang, Jiang, and Gusfield recently improved the efficiency of their PTAS for tree alignment [16], but still use dynamic programming.

We give a simple 2-approximation for the fixed-topology  $\ell$ -phylogeny problem that works for arbitrary input topologies. It is based on rounding the linear-programming relaxation of an integer programming formulation for the fixed-topology  $\ell$ -phylogeny problem. To our knowledge, this is the first application of linear-programming technology to phylogeny problems.

As we described earlier,  $\ell$ -phylogeny is most appropriate for slowly-evolving characters. It is most restrictive (and hence most different from parsimony) when  $\ell$  is small. Therefore, we look more closely at the first *NP*-hard case:  $\ell = 3$ . For this case, we give an algorithm based upon the structure of a 3-phylogeny that will construct a 4-phylogeny if the input instance has a 3-phylogeny.

The remainder of our paper is organized as follows: in section 2, we give the 2-approximation algorithm for the  $\ell$ -phylogeny problem. In section 3 we give the optimal approximation algorithm for inputs with 3-phylogenies. In section 4, we extend the linear-programming-based techniques to develop an approximation algorithm for the problem of finding parsimonious low-load labellings for phylogenies with polymorphic characters.

**2. A 2-approximation algorithm for the fixed-topology phylogenetic number problem.** The interaction between characters in phylogeny problems affects the choice of the topology, but it does not affect the labelling of the internal nodes once the topology is chosen. Thus, for this problem, we can consider each character separately.

Let  $c : S \rightarrow \{1, \dots, r\}$  be a character and let  $T$  be a tree with root  $q$  and leaves labelled by character states  $1, \dots, r$ . For each state  $i$ , let  $T_i$  be the subtree of  $T$  consisting of all the leaves labelled  $i$  and the minimum set of edges connecting these leaves. Let  $L(T_i)$  be the set of leaves of  $T_i$ , and let  $rt_i$ , the root of  $T_i$ , be the node of  $T_i$  closest to the root of  $T$ . The *important nodes* of  $T_i$  are the leaf nodes and the nodes of degree greater than 2. An  *$i$ -path*  $p$  of  $T_i$  is a sequence of edges of  $T_i$  that connects two important nodes of  $T_i$ , but does not pass through any other important nodes. The two important nodes are referred to as the *endpoints* of  $p$ , and the other nodes along the  $i$ -path are said to be *on*  $p$  (an  $i$ -path need not have any nodes on it). Although the edges of the tree  $T$  are undirected, we will sometimes use the notation  $(v \rightarrow w)$  for an edge or  $i$ -path with endpoints  $v$  and  $w$ , to indicate that  $v$  is nearer to the root of  $T$  than  $w$  ( $v$  is the *higher* endpoint and  $w$  is the *lower* endpoint); otherwise we will write edges and  $i$ -paths as  $(v, w)$ . If the lower endpoint  $w$  is labelled  $i$  and the label of the upper endpoint  $v$  or some node on the  $i$ -path  $p = (v \rightarrow w)$  is not  $i$ , then we say that  $p$  *breaks* state  $i$ . If an  $i$ -path goes through the (degree-2) root of  $T_i$ , then *both* endpoints are considered lower endpoints.

Given a tree  $T$  with each node labeled from the set  $\{1, \dots, r\}$ , we need a way to count the number of components induced by the nodes labeled  $i$ . Since the tree is rooted, we can assign each connected component a root, namely the node closest to the root of  $T$ . We then count the number of roots for components labelled  $i$ . A node is the root of its component if its label differs from that of its parent. The root  $q$ , which has no parent, is also the root of its component. Therefore we have the following:

**OBSERVATION 2.1.** *Let  $T$  be a tree with its leaves and internal nodes labelled by elements of  $\{1, \dots, r\}$ . For each  $i$ , let  $T_i$  be defined as above, and let  $q$  be the root of tree  $T$ . Then the number of connected components induced by the nodes labelled  $i$  is  $|\{e = (v \rightarrow w) : c(v) \neq i, c(w) = i\}| + Y_i$ , where  $Y_i = 1$  if  $q$  is labelled  $i$  and 0 otherwise.*

We now define an integer linear program (ILP) which solves the fixed-topology  $\ell$ -phylogeny problem. The linear-programming relaxation of this ILP is the key to our 2-approximation algorithm. The integer linear program  $\mathcal{I}$  uses the variables  $X_{v,i}$ , for each state  $i \in \{1, \dots, r\}$ , and each node  $v$  in the tree  $T$ , the variables  $X_{p,i}$  for each state  $i$ , and each  $i$ -path  $p$  of  $T_i$  and the variables  $cost_{p,v,i}$  for each state  $i$ ,  $i$ -path  $p$  in  $T_i$  and each lower endpoint  $v$  of path  $p$ . Recall that each path has one lower endpoint except when there is an  $i$ -path through a degree-2 root, in which case both endpoints are lower endpoints. These variables have the following interpretation:

$$\begin{aligned}
X_{v,i} &= \begin{cases} 1 & \text{if node } v \text{ is labelled } i \\ 0 & \text{otherwise} \end{cases} \\
X_{p,i} &= \begin{cases} 1 & \text{if all nodes on } p \text{ are labelled } i \\ 0 & \text{otherwise} \end{cases} \\
cost_{p,v,i} &= \begin{cases} 1 & \text{if lower endpoint } v \text{ of } p \text{ is the root of a component of state } i \\ 0 & \text{otherwise} \end{cases}
\end{aligned}$$

ILP  $\mathcal{I}$  is defined as follows:

minimize  $\ell$

subject to

- (1)  $X_{v,i} = 1$  for each leaf  $v \in T_i$ ,  $i = 1, \dots, r$
- (2)  $X_{v,i} = 0$  if  $v \notin T_i$ ,  $i = 1, \dots, r$
- (3)  $\sum_{i=1}^r X_{v,i} \leq 1$   $\forall v \in T$
- (4)  $X_{p,i} = X_{v,i}$   $i = 1, \dots, r, \forall p \in T_i, \forall v \in p$
- (5)  $X_{p,i} \leq X_{v,i}$   $i = 1, \dots, r, \forall p \in T_i, \text{endpoint } v \in p$
- (6)  $cost_{p,v,i} \geq X_{v,i} - X_{p,i}$   $i = 1, \dots, r, \forall p \in T_i, \text{lower endpoint } v \in p$
- (7)  $\sum_{p,v} cost_{p,v,i} + X_{rt_i,i} \leq \ell$   $i = 1, \dots, r$
- (8)  $X_{v,i}, X_{p,i}, cost_{p,v,i} \in \{0, 1\}$

Constraint (8) assures that the cost ( $cost_{p,v,i}$ ),  $i$ -path ( $X_{p,i}$ ), and vertex ( $X_{v,i}$ ) variables serve as indicator variables in accordance with their interpretation. Constraint (1) labels the leaves in accordance with the input. Constraint (2) prohibits labelling a node  $v$  with a state  $i$  when  $v$  is not in  $T_i$  (the number of components labelled  $i$  could not possibly be reduced by this labelling). Constraint (3) ensures that each internal node will have no more than one label. Constraints (4) and (5) ensure that for each tree  $T_i$ , nodes on paths are taken all-or-none; if any node on an  $i$ -path  $p$  (including endpoints) is lost to a state  $i$ , then it does no good to have any of the other nodes on the path (though it may be beneficial to maintain one or both endpoints). Constraint (6) computes the path costs (counts roots) and constraint (7) ensures that each state has no more than  $\ell$  connected components. This is an implementation of Observation 2.1. Since there is no  $i$ -path in  $T_i$  with  $rt_i$  as its lower endpoint, we must explicitly check the root of each tree  $T_i$ , just as we checked the global root in Observation 2.1.

Integer program  $\mathcal{I}$  solves the fixed-topology  $\ell$ -phylogeny problem. We will now show that the optimal value of  $\ell$  given by  $\mathcal{I}$  is a lower bound on the phylogenetic number of tree  $T$  with the given leaf labelling.

**PROPOSITION 2.2.** *If there exists an  $\ell$ -phylogeny for tree  $T$  with a given leaf labelling, then there is a feasible solution for the integer linear program for this value of  $\ell$ .*

*Proof.* Suppose there exists an  $\ell$ -phylogeny on the tree  $T$  with leaves and internal nodes labelled from  $\{1, \dots, r\}$ . Consider one particular  $\ell$ -phylogeny, and assume without loss of generality that all node labels are useful for connectivity (i.e. changing

the label of node  $v$  from  $i$  to something else will increase the number of components labelled  $i$ ). This may require some nodes to be unlabelled. We obtain a feasible solution to  $\mathcal{I}$  as follows. Set variable  $X_{v,i}$  to 1 if node  $v$  is labelled  $i$  in this phylogeny and 0 otherwise. Set  $X_{p,i}$  to 1 if both endpoints and all internal nodes of  $i$ -path  $p$  are labelled  $i$  and 0 otherwise. Set  $cost_{p,v,i} = 1$  if lower endpoint  $v$  of  $p$  is labelled  $i$  and the  $i$ -path is not, and set  $cost_{p,v,i} = 0$  otherwise. We now show this assignment is a solution to  $\mathcal{I}$ .

The  $X_{v,i}$ ,  $X_{p,i}$ , and  $cost_{p,v,i}$  variables are binary by construction, thus satisfying Constraint (8). By construction, Constraint (1) will be satisfied by our assignment. Constraint (2) will also be satisfied, because it is never useful to label nodes outside  $T_i$  with  $i$ , and we have assumed all the labels on nodes are useful for connectivity. Constraint (3) is also satisfied because each node of the phylogeny will be labelled with at most one state. Constraints (4) and (5) are satisfied because the condition that all labelled nodes are necessary for connectivity ensures that a node on an  $i$ -path will only be labelled  $i$  if all the nodes and endpoints of the  $i$ -path are labelled  $i$ . Constraint (6) is satisfied by construction.

To show that constraint (7) is satisfied, consider the connected components for  $i$ ; by our assumption, these all lie in  $T_i$ . Let  $\gamma = \{e = (v \rightarrow w) : c(v) \neq i, c(w) = i\}$ . By Observation 2.1 we have  $|\gamma| + X_{q,i} \leq \ell$ , where  $q$  is the root of  $T$ . To calculate  $(\sum_{p,v} cost_{p,v,i}) + X_{rt_i,i}$ , note that  $cost_{p,w,i} = 1$  if and only if  $X_{w,i} = 1$  for the lower endpoint  $w$  and  $X_{p,i} = 0$  and otherwise  $cost_{p,w,i}$  is 0. By our definitions above,  $X_{p,i} = 0$  and  $X_{w,i} = 1$  if and only if the edge  $(v, w) \in T$  from  $w$ 's parent (on the  $i$ -path  $p$  or its upper endpoint) into  $w$  has  $c(v) \neq i$  and  $c(w) = i$ . Furthermore, this is the only edge on the  $i$ -path with this property (the cost of each other edge is 0) unless path  $p$  passes through a degree-2 root and both its endpoints have breaks. In the latter case there is a second endpoint  $w'$  such that  $cost_{p,w',i} = 1$ . Since the  $i$ -paths partition  $T_i$ , each  $i$ -path  $p$  and lower endpoint  $v$  with  $cost_{p,v,i} = 1$  contains one element of  $\gamma$  which is unique to that  $i$ -path and lower endpoint. Thus  $(\sum_{p,v} cost_{p,v,i}) \leq |\gamma| \leq \ell$ . If  $rt_i$  is the node  $q$ , then  $X_{rt_i,i} = X_{q,i}$  and  $(\sum_{p,v} cost_{p,v,i}) + X_{rt_i,i} \leq |\gamma| + X_{q,i} \leq \ell$ . Otherwise, if  $rt_i$  is not the global root  $q$ , by our assumption that only useful nodes of  $T$  are labelled with  $i$ , the ancestor node  $a_i$  of  $rt_i$  is not labelled  $i$ . Then, if  $X_{rt_i,i} = 1$  the edge  $e = (a_i \rightarrow rt_i)$  contributes 1 to  $|\gamma|$ , and therefore  $(\sum_{p,v} cost_{p,v,i}) + X_{rt_i,i} \leq |\gamma| + X_{q,i} \leq \ell$ . Hence constraints (7) are satisfied and we have a solution for the integer program  $\mathcal{I}$ .  $\square$

Integer linear programming in  $\mathcal{NP}$ -hard in general [3, 10, 12], so we cannot solve it directly in polynomial time. (In fact, doing so would solve the fixed-topology  $\ell$ -phylogeny problem, which we know to be  $\mathcal{NP}$ -hard for  $\ell \geq 3$  from [9].) However, we can solve the linear-programming relaxation  $\mathcal{L}$  of  $\mathcal{I}$ , which consists of all the constraints of  $\mathcal{I}$  except that Constraint (8) is replaced by the constraint  $0 \leq X_{v,i}, X_{p,i}, cost_{p,v,i} \leq 1$  (8'). Note that the right-hand side of constraint (6) could be negative, but the relaxed version of the constraint (8) is still sufficient to prevent the path cost variables from being negative.

**THEOREM 2.3.** *If there is a solution for the linear program  $\mathcal{L}$  for a fixed topology  $T$  with leaves labelled with states from  $\{1, \dots, r\}$ , then we can assign states to the internal nodes of  $T$  such that no state  $i \in \{1, \dots, r\}$  has more than  $2\ell$  components.*

*Proof.* The  $2\ell$  phylogeny for the character  $c : S \rightarrow \{1, \dots, r\}$  on  $T$  is constructed by assigning states to the nodes of each tree  $T_i$  based on the  $X_{v,i}$  values. For each state  $i \in \{1, \dots, r\}$ , consider each internal node  $v$  of  $T_i$ . A node  $v$  is labelled  $i$  if and only if  $X_{v,i} > 1/2$ , and there is a path  $v, w_1, w_2, \dots, w_k, v^*$  through tree  $T_i$  to a leaf

$v^*$  of  $T_i$  where  $X_{w_j,i} > 1/2$  for all  $j = 1, \dots, k$ . If  $X_{v,i} > 1/2$ , but there is no such path, then node  $v$  is *isolated*, and by our procedure remains unlabelled. A node  $v$  also remains unlabelled if  $X_{v,i} \leq 1/2$  for all states  $i$ .

To show that the labelling is a  $2\ell$ -phylogeny, we show that each component of state  $i$  adds at least  $1/2$  to the sum  $(\sum_{p,v} \text{cost}_{p,v,i}) + X_{rt_i,i}$ . From Observation 2.1, the number of connected components for the state  $i$  is  $|\{e = (v \rightarrow w) : c(v) \neq i, c(w) = i\}| + Y_i$ , where  $Y_i$  is 1 if  $q$  has state  $i$  (and therefore  $q = rt_i$ ) and 0 otherwise. Constraints (5) and (4) ensure that if the edge  $e = (v \rightarrow w)$  has  $c(v) \neq i$  and  $c(w) = i$  then either  $w$  is the root of  $T_i$ , or  $w$  must be an endpoint node with  $X_{w,i} > 1/2$ , and that either  $X_{v,i} \leq 1/2$  or  $v$  is isolated. However, since  $w$  is labelled  $i$ ,  $w$  must not be isolated, and therefore  $v$  would not be isolated if  $X_{v,i}$  was greater than  $1/2$ . So  $X_{v,i} \leq 1/2$ , and  $X_{p,i} \leq 1/2$  for the  $i$ -path  $p$  with lower endpoint  $w$ . Therefore we need only calculate the number of lower endpoints  $w$  from  $i$ -paths  $p$  such that  $X_{p,i} \leq 1/2$ ,  $X_{w,i} > 1/2$ , and  $w$  is not isolated.

Suppose  $w$  is a lower endpoint of  $i$ -path  $p$ . Since  $w$  is not isolated and the node above  $w$  is not labelled  $i$ , there is a sequence  $p_1 = (w \rightarrow v_1)$ ,  $p_2 = (v_1 \rightarrow v_2), \dots, p_j = (v_{j-1} \rightarrow v_j)$  of  $i$ -paths of  $T_i$  such that  $X_{p,i} > 1/2$  for every  $p \in \{p_1, \dots, p_j\}$  and  $X_{v,i} > 1/2$  for every  $v \in \{v_1, \dots, v_j\}$ , and  $v_j$  is a leaf of  $T_i$ . Calculating  $\text{cost}_{p,w,i} + \text{cost}_{p_1,v_1,i} + \dots + \text{cost}_{p_j,v_j,i} = (X_{w,i} - X_{p,i}) + (X_{v_1,i} - X_{p_1,i}) + \dots + (X_{v_j,i} - X_{p_j,i}) = -X_{p,i} + (X_{w,i} - X_{p_1,i}) + (X_{v_1,i} - X_{p_2,i}) + \dots + (X_{v_{j-1},i} - X_{p_j,i}) + X_{v_j,i}$ , we know by constraints (5) that  $X_{w,i} - X_{p_1,i} \geq 0$ ,  $X_{v_1,i} - X_{p_2,i} \geq 0$ ,  $\dots$ ,  $X_{v_{j-1},i} - X_{p_j,i} \geq 0$ . So  $\text{cost}_{p,w,i} + \text{cost}_{p_1,v_1,i} + \dots + \text{cost}_{p_j,v_j,i} \geq X_{v_j,i} - X_{p,i} = 1 - X_{p,i} \geq 1/2$ .

Note that for any two breaks that appear at lower endpoints  $w$  and  $w'$  of  $i$ -paths  $p$  and  $p'$  respectively, the  $i$ -labelled paths to leaves are disjoint (because they are in separate components of  $i$ ). Therefore each break of  $i$  at a lower endpoint  $w$  contributes at least  $1/2$  to the sum  $(\sum_{p,v} \text{cost}_{p,v,i})$ . If  $rt_i$  is labelled  $i$  (and hence the root of a component of  $i$ ), then  $X_{rt_i,i} > 1/2$  (corresponding to an edge  $(v \rightarrow rt_i)$  in  $T$  or to the case  $Y_i = 1$ ). So  $2 \times ((\sum_{p,v} \text{cost}_{p,v,i}) + X_{rt_i,i}) \geq |\{e = (v \rightarrow w) : c(v) \neq i, c(w) = i\}| + Y_i$ , and therefore  $2\ell \geq |\{e = (v \rightarrow w) : c(v) \neq i, c(w) = i\}| + Y_i$ .  $\square$

Theorem 2.3 is tight as shown by the following example: let the input topology be a star graph with  $2x$  leaves:  $x$  leaves labelled  $i$  and  $x$  labelled  $j$ . The LP solution has the root labelled half  $i$  and half  $j$ , so that  $\ell = (x + 1)/2$  by constraint 6. The optimal solution has  $\ell = x$ , arbitrarily close to twice the LP bound. In this example, however, it is the LP bound which is loose, and therefore our analysis of the approximation quality of the algorithm may not be tight.

Recall that we have considered each character separately in our 2-approximation algorithm. Thus, our work applies to the generalized  $\ell$ -phylogeny problem (and not just to the ordinary  $\ell$ -phylogeny problem). In particular, we have the following theorem.

**THEOREM 2.4.** *There is a 2-approximation algorithm for the generalized  $\ell$ -phylogeny problem.*

**3. 4-phylogeny algorithm.** In this section we give an algorithm which takes a fixed-topology phylogeny instance with arbitrary topology and, as long as it has a 3-phylogeny, finds a 4-phylogeny for the instance.

We use the following definitions, in addition to those that we used for the 2-approximation. We will maintain a forest  $F_i$  for every state  $i$ , which corresponds to



the set of nodes that state  $i$  is contending for. A **branch point** of  $F_i$  is a node in  $F_i$  with degree 3. We say that a node  $v \in F_i$  is *claimed* by state  $i$  if it is not in  $F_j$  for any  $j \neq i$ .

The algorithm generalizes the fixed-topology 2-phylogeny algorithm of [9]. It consists of a *forced phase* and then an *approximation phase*. The forced phase produces a partial labelling (resolution of labels on some subset of the nodes) which can still be extended to a 3-phylogeny; it makes no labelling decisions that are not forced if one is to have a 3-phylogeny. The approximation phase removes all remaining contention for labels, but it can break some states into four pieces. Because finding a fixed-topology 3-phylogeny is  $\mathcal{NP}$ -complete [9], this is an optimal approximation algorithm for phylogeny instances with 3-phylogenies.

**3.1. The Forced Phase of the Algorithm.** Initially, for every state  $i$  we will have  $F_i = T_i$ . During the forced phase of the algorithm, nodes will be removed from the forests  $F_i$ . The invariant during the forced phase of the algorithm is that there is a 3-phylogeny in which every node  $v$  is assigned a state  $j$  such that  $v \in F_j$ . The forced phase applies the following rules in any order until none can be applied. If any forest  $F_i$  is broken into more than three components by the application of these rules, then the instance has no 3-phylogeny and the algorithm terminates.

1. For any  $i$ -path  $(v, w)$ , let  $S$  be the set containing  $v$  and  $w$  and the nodes on the  $i$ -path. If  $S$  contains two or more branch points of  $F_j$  (for  $i \neq j$ ) then every node on the  $i$ -path is removed from  $F_i$ . Note that in the updated copy of  $F_i$  (after the rule is applied),  $v$  and  $w$  will have lower degree than in the original  $F_i$ . Furthermore, if  $v$  has degree 2 in the updated  $F_i$  then the  $i$ -path containing it will consist of nodes from two different  $i$ -paths in the original  $F_i$ . Similarly,  $i$ -paths can be merged as a result of the following rules.
2. If  $F_i$  has  $C(F_i)$  connected components and  $F_i$  contains a node  $v$  of degree at least  $5 - C(F_i)$  then in every forest  $F_j$  with  $j \neq i$ ,  $v$  and all nodes on  $j$ -paths adjacent to  $v$  are removed from  $F_j$  (i.e.,  $i$  claims node  $v$ ).
3. Suppose  $v$  is a branch point of  $F_i$  but not a branchpoint of  $F_j$ , and suppose two  $i$ -paths  $(v, w_1)$  and  $(v, w_2)$  adjacent to  $v$  each contain a branch point of  $F_j$ . Then in every forest  $F_k$  with  $k \neq i$ , every branch point  $w \notin \{v, w_1, w_2\}$  of  $F_i$  and every node on every  $k$ -path adjacent to  $w$  is removed from  $F_k$  (i.e.,  $F_i$  claims all branchpoints except  $v$ ,  $w_1$ , and  $w_2$ ).

Rule 1 is justified by observing that in any 3-phylogeny, each forest  $F_i$  gives up at most two disjoint  $i$ -paths, or a single branchpoint with the  $i$ -paths adjacent to it. In the setting in which rule 1 is applied, if  $F_i$  were to claim the path in question, then  $F_j$  would lose two branchpoints and necessarily be in at least four components. Therefore, in any 3-phylogeny for the input,  $F_i$  cannot have that  $i$ -path. Note that once any node on an  $i$ -path is lost to  $F_i$ , then  $F_i$  has no reason to claim any other nodes on the  $i$ -path.

Rule 2 is justified by the following observations. If there is a node of degree at least 4 in tree  $T_i$ , then it must be labelled  $i$  in any 3-phylogeny (losing it will break state  $i$  into at least 4 pieces). Once  $F_i$  has been forced to give up an  $i$ -path, it cannot give up another branchpoint. Finally, once  $F_i$  has been forced into three pieces, then it must claim all remaining nodes in  $F_i$ .

Rule 3 is applied when we isolate a region where a break in  $F_i$  must occur, but do not yet know exactly where the break will occur. If two paths adjacent to a branchpoint

of  $F_i$  contain branchpoints of  $F_j$ , then by the previous argument for rule 1,  $F_i$  cannot keep both of those paths. Therefore, outside of the affected region (those two  $i$ -paths),  $F_i$  can act as though the forest has been cut into at least two pieces, and can claim all branchpoints.

**3.2. The Approximation Phase of the Algorithm.** In the following, *releasing* a degree-2 node  $v \in F_i$  removes all nodes on its  $i$ -path from  $F_i$ . Releasing a higher-degree node  $v \in F_i$  removes  $v$  and all nodes on  $i$ -paths adjacent to  $v$  from  $F_i$ . The approximation phase consists of the following steps.

1. For each connected component  $C$  of  $F_i$ , if the root of  $C$  is unclaimed then  $F_i$  releases the root of  $C$ . Also, if this root has degree 2,  $F_i$  releases any unclaimed branch points at the ends of the  $i$ -path through this root.
2. If, after the forced phase,  $F_i$  is in a single component with exactly one unclaimed branch point,  $w$ , then it releases  $w$ .
3. If, after the forced phase,  $F_i$  is in a single component with exactly two unclaimed branch points,  $w_1$  and  $w_2$  which are the two endpoints of an  $i$ -path, and the path from the root to  $w_2$  passes through  $w_1$ , then  $F_i$  releases  $w_2$ .
4. If, after the forced phase,  $F_i$  is in a single component with exactly three unclaimed branch points,  $w_1$ ,  $w_2$  and  $w_3$  where there is an  $i$ -path from  $w_1$  to  $w_2$  and an  $i$ -path from  $w_2$  to  $w_3$ , then  $F_i$  releases  $w_2$ .

**3.3. The Proof of Correctness.** The proof of correctness of the algorithm requires the following observation, and follows from Lemma 3.2 and Lemma 3.7.

**OBSERVATION 3.1.** *If  $F_i$  is in one component and it releases two branchpoints  $w_1$  and  $w_2$  which share an  $i$ -path, then the resulting forest  $F_i$  has at most 4 components.*

*Proof.* Suppose without loss of generality that branchpoint  $w_1$  is removed first. This leaves  $F_i$  in three pieces. Because  $w_2$  shares an  $i$ -path with  $w_1$ , this operation reduces the degree of  $w_2$  to two, so the two remaining  $i$ -paths adjacent to  $w_2$  are merged. Subsequently removing the  $i$ -path through  $w_2$  adds only one more component.  $\square$

**LEMMA 3.2.** *At the end of the approximation phase, every forest  $F_i$  has at most 4 connected components.*

*Proof.* The forest  $F_i$  can be in at most three components at the end of the forced phase. If  $F_i$  is in three components at the end of the forced phase, then, by Rule 2 of the forced phase, every remaining node in  $F_i$  is claimed during the forced phase, so nothing is removed from  $F_i$  during the approximation phase. If  $F_i$  is in two components after the forced phase, then, again by Rule 2, all branch points of  $F_i$  are claimed during the forced phase, so no branch points are removed from  $F_i$  during the approximation phase. Step 1 of the approximation phase, therefore, will remove at most one path from each component (when the root has degree 2, since degree-3 roots are claimed) and therefore breaks  $F_i$  into at most four components. In this case Steps 2–4 of the approximation phase do not apply, and at most one of Steps 2–4 can apply to each of the remaining cases.

If  $F_i$  is in one component after the forced phase, and Steps 2–4 do not apply then we have two cases. If the root is degree three, Step 1 results in at most 3 components. If the root is degree two, then  $F_i$  could release the two branchpoints on either end of this  $i$ -path, resulting in at most four components by Observation 3.1.

Suppose  $F_i$  is in one component with exactly one unclaimed branchpoint after the forced phase. If that branchpoint is released by Step 1, then  $F_i$  is in at most

3 components after that step (only that branchpoint and its adjacent  $i$ -paths are removed from  $F_i$ ), and Step 2 is redundant. Otherwise, Step 1 only has an effect if the root has degree 2. In this case, Step 1 releases only the  $i$ -path through the root, since its endpoints are claimed, resulting in two components, and the subsequent application of Step 2 adds at most two more for a total of four.

Suppose Step 3 can be applied to  $F_i$ . If  $w_1$  is not an endpoint of the  $i$ -path through the root of  $F_i$  (or the root itself), then, as in the previous case, Step 1 results in at most two components. Subsequently removing  $w_2$  by Step 3 results in at most two more components for a total of four. If  $w_1$  is an endpoint of the  $i$ -path containing the root of  $F_i$  (or the root itself), then both  $w_1$  and  $w_2$  are released (and nothing more). Since they share an  $i$ -path, this results in at most four components by Observation 3.1.

Finally, suppose Step 4 can be applied to  $F_i$ . If none of  $w_1, w_2$  or  $w_3$  is the root or is an endpoint of the  $i$ -path adjacent to the root, then Step 1 will result in additional components only if the root has degree two. Since both of the endpoints of this  $i$ -path are claimed in this case, removing this  $i$ -path and  $w_2$  (by Step 4) results in at most four components. Otherwise, the combined application of Steps 1 and 4 requires the release of  $w_2$ , and possibly one of  $w_1$  and  $w_3$  as well (but not both, since if  $w_2$  is the root, neither of the other branchpoints will be released). By Observation 3.1 this will result in at most four components.  $\square$

The following lemmas use this fact:

FACT 3.3. ([9]) *The intersection of two subtrees of a tree is connected and contains the root of at least one of the subtrees.*

LEMMA 3.4. *If  $F_i$  and  $F_j$  are each in two components after the forced phase, then after the approximation phase, there is no node that is in  $F_i$  and in  $F_j$ .*

*Proof.* This proof is similar to the correctness proof of the fixed-topology 2-phylogeny algorithm in [9]. Let  $C_i$  be a component of  $F_i$  after the forced phase, and let  $C_j$  be a component of  $F_j$  after the forced phase. Since  $F_i$  and  $F_j$  are both split in two components during the forced phase, all branch points in  $C_i$  and  $C_j$  are claimed during the forced phase (by Rule 2), and their intersection is a path in the fixed topology (i.e., all nodes are degree 2). Furthermore, the root of  $C_i$  or  $C_j$  is in the intersection. Therefore, the contention is cleared in Step 1 of the approximation phase of the algorithm.  $\square$

LEMMA 3.5. *If  $F_i$  is in one component after the forced phase, and  $F_j$  is in two components after the forced phase, then there is no node that is in  $F_i$  and in  $F_j$  after the approximation phase.*

*Proof.* First note that no branch point of  $T_j$  is part of  $T_i$ . (Since  $F_j$  is in only 2 pieces, it gave up only degree-2 nodes in the forced phase, and subsequently claimed all branch points. None of these are in  $F_i$ , since  $F_i$  was unbroken in the forced phase). Thus, the intersection of  $T_i$  and  $T_j$  is a path in  $T_j$ . We conclude that the intersection of  $F_i$  and  $F_j$  is a path in  $F_j$  and contains at most one branch point of  $F_i$  (otherwise, the path would be removed from  $F_j$  during the forced phase by Rule 1). If the intersection contains the root of  $F_j$ , then the contention will be removed during Step 1 of the approximation phase. Otherwise, the intersection contains the root of  $F_i$ . Thus, the single branch point of  $F_i$  that is contained in the intersection of  $F_i$  and  $F_j$  is either the root of  $F_i$  or it is an endpoint of the  $i$ -path containing the root of  $F_i$ . In either case, the contention will be removed in Step 1 of the approximation phase.  $\square$

LEMMA 3.6. *If  $F_i$  and  $F_j$  are each in one component after the forced phase, then there is no node that is in  $F_i$  and in  $F_j$  after the approximation phase.*

*Proof.* We will consider various cases. Case  $(\alpha, \beta, \gamma)$  will represent the situation in which the intersection of  $F_i$  and  $F_j$  after the forced phase contains  $\alpha$  branch points of  $F_i$  and  $\beta$  branch points of  $F_j$ ,  $\gamma$  of which are shared. Recall that when a branchpoint  $v$  of  $F_i$  is released,  $v$  and all nodes on  $i$ -paths adjacent to  $v$  are removed from  $F_i$ .

**Case  $(0, 0, 0)$ :** As in the proof of Lemma 3.4, the intersection of  $F_i$  and  $F_j$  is a path containing the root of one of  $F_i$  and  $F_j$ , so the contention is cleared in Step 1 of the approximation phase.

**Case  $(1, 0, 0)$ :** As in the proof of Lemma 3.5, the intersection of  $F_i$  and  $F_j$  is a path of  $F_j$  containing one branch point of  $F_i$  so the contention is cleared in Step 1 of the approximation phase.

**Case  $(1, 1, \gamma)$ :** Suppose without loss of generality that the root of  $F_i$  is in the intersection of  $F_i$  and  $F_j$  after the forced phase. Then the branch point of  $F_i$  is either the root of  $F_i$  or it is the endpoint of an  $i$ -path containing the root of  $F_i$ . In either case, it is released by  $F_i$  during Step 1 of the approximation phase.

**Case  $(2, 0, 0)$ :** This case cannot arise after the forced phase, because it requires two branch points of  $F_i$  on a single path of  $F_j$ , which is forbidden by Rule 1 of the forced phase.

**Case  $(2, 1, 0)$ :** By Rule 1, after the forced phase, the intersection of  $F_i$  and  $F_j$  has the branchpoint of  $F_j$  ( $w_2$ ), between the two branchpoints for  $F_i$  ( $w_1$  and  $w_3$ ) as illustrated in Figure 2(a). Let  $w_4$  be the other endpoint of the  $j$ -path adjacent to  $w_2$  that contains  $w_1$ , and let  $w_5$  be the other endpoint of the  $j$ -path adjacent to  $w_2$  that contains  $w_3$ . By Rule 3 of the forced phase, all branch points of  $F_j$  except  $w_2$ ,  $w_4$  and  $w_5$  are claimed. If node  $w_2$  is released by  $F_j$  during the approximation phase, then the contention is cleared. Otherwise, by Rules 2 and 4 of the approximation phase, exactly one of  $\{w_4, w_5\}$  is unclaimed after the forced phase. Suppose without loss of generality this is  $w_4$ . Because  $w_2$  is not released by  $F_j$  in the approximation phase, the root of  $F_j$  is not  $w_2$  or on any  $j$ -path adjacent to it. Therefore the root of  $F_i$  is in the intersection. If the root of  $F_i$  is on the  $i$ -path between  $w_1$  and  $w_3$  then by Step 1 of the approximation phase,  $F_i$  will release both  $w_1$  and  $w_3$ , and the contention will be cleared. If the root of  $F_i$  was on the other  $i$ -path adjacent to  $w_1$  in the intersection, then  $w_4$  would be the closest to the root of  $F_j$  among the three unreleased  $F_j$  branchpoints, and  $F_j$  would have released  $w_2$  by step 3 of the approximation phase. Finally, if the root is on an  $i$ -path adjacent to  $w_3$  (but not  $w_1$ ),  $F_i$  will release  $w_3$  by Step 1 of the approximation phase, clearing the  $i$ -path from  $w_3$  to  $w_1$  (not including  $w_1$ ). By Step 3 of the approximation phase  $F_j$  will release  $w_4$ , clearing the  $j$ -path from  $w_2$  to  $w_4$  (not including  $w_2$ ). Therefore the contention is removed.

**Case  $(2, 1, 1)$ :** This case cannot arise after the forced phase, because it requires two branch points of  $F_i$  on a single path (including endpoints) of  $F_j$ , which is forbidden by Rule 1 of the forced phase.

**Case  $(2, 2, 0)$ :** By Rule 1 of the forced phase, the branch points of  $F_i$  and  $F_j$  are interleaved and lie on a path, as illustrated in Figure 2(b). Label the four relevant branch points  $w_1, w_2, w_3, w_4$  such that for  $k \in \{1, 2, 3\}$ , there is a path between  $w_k$  and  $w_{k+1}$  which does not pass through any  $w_\ell \notin \{w_k, w_{k+1}\}$ . Without loss of generality, assume that  $w_1$  is a branch point of  $F_i$ . Let  $w_5$  be the other endpoint of the  $j$ -path adjacent to  $w_2$  that contains  $w_1$ , and let  $w_6$  be the other end of the  $i$ -path adjacent to  $w_3$  that contains  $w_4$ . By repeated applications of Rule 3 of the forced phase, all branch points of  $F_i$  and  $F_j$  other than  $w_1$ – $w_6$  are claimed.

If  $F_j$  does not claim  $w_5$  in the forced phase and  $F_i$  does not claim  $w_6$ , then by

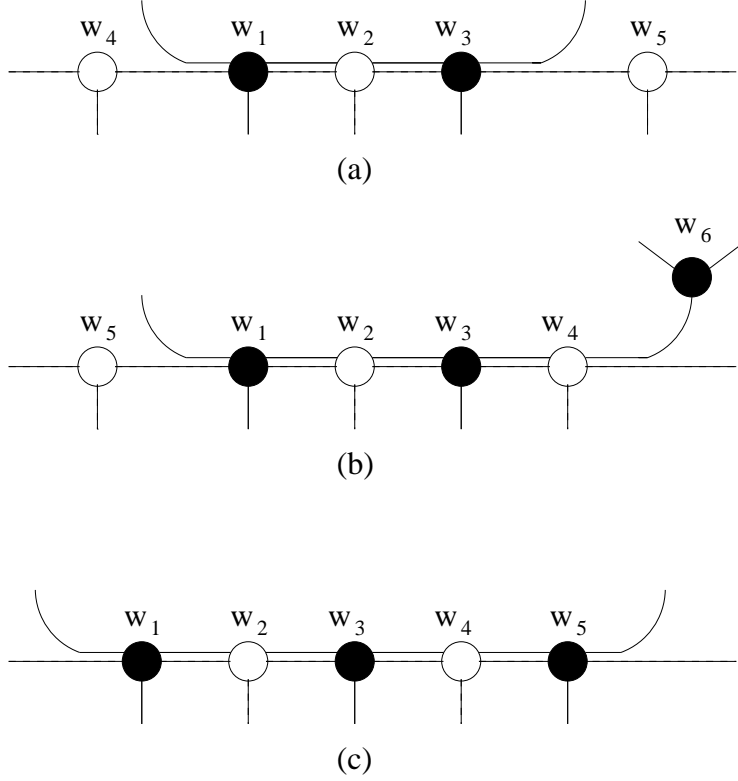


FIG. 2. Cases from Lemma 10. Branchpoints of forest  $F_i$  are represented by solid circles, and  $i$ -paths are solid lines. Branchpoints of forest  $F_j$  are represented as empty circles with  $j$ -paths as dashed lines. Dashed and solid together represent shared paths. (a) case  $(2, 1, 0)$ , (b) case  $(2, 2, 0)$ , and (c) case  $(3, 2, 0)$ .

Rule 4 of the approximation phase,  $w_3$  is released by  $F_i$  and  $w_2$  is released by  $F_j$ , so the contention is cleared.

So, suppose without loss of generality that  $w_6$  is claimed by  $F_i$ . Consider the location of the root of  $F_i$  relative to  $w_1$  and  $w_3$ . If the root of  $F_i$  is on the far side of  $w_6$  (down one of the  $i$ -paths not adjacent to  $w_3$ ), or on the  $(w_3, w_6)$   $i$ -path between  $w_4$  and  $w_6$ , then  $w_4$  is on a  $j$ -path adjacent to the root of  $F_j$ . Therefore, by Step 1 of the approximation phase,  $F_j$  will release  $w_4$ , clearing contention up to, but not including  $w_2$ , and by Step 3 of the approximation phase,  $F_i$  will release  $w_1$ , clearing the remaining contention. A similar argument holds when the root is on the far side of  $w_1$ . If the root is on the  $(w_1, w_3)$   $i$ -path, then by Step 1 of the approximation phase,  $F_i$  releases both  $w_1$  and  $w_3$ , removing contention. Similarly, if the root is on the  $(w_2, w_4)$   $j$ -path, (included in  $F_i$ ), then  $F_j$  releases both  $w_2$  and  $w_4$ .

**Case  $(3, 2, 0)$ :** By Rule 1 of the forced phase, the branch points of  $F_i$  and  $F_j$  are interleaved and lie on a path as illustrated in Figure 2(c). Label the five relevant branch points  $w_1, w_2, w_3, w_4, w_5$  such that for  $k \in \{1, 2, 3, 4\}$ , there is a path between  $w_k$  and  $w_{k+1}$  which does not pass through any  $w_\ell \notin \{w_k, w_{k+1}\}$ . By repeated application of Rule 3 of the forced phase, all branch points of  $F_i$  and  $F_j$  other than  $w_1$ – $w_5$  are claimed. Node  $w_3$  is released by  $F_i$  by Rule 4 of the approximation phase. Contention remains at  $w_1$  and  $w_5$ . Consider where the global root is with respect to this intersection. If the global root is located down one of the paths adjacent to  $w_1$  (but not adjacent to  $w_3$ ), then the root of  $F_j$  is on an  $j$ -path adjacent to  $w_2$ .  $F_j$  releases  $w_2$  by Step 1 of

the approximation phase and  $w_4$  by Step 3 of the approximation phase, removing the remaining contention. A similar argument holds if the root is down a  $i$ -path adjacent to  $w_5$  (other than  $(w_3, w_5)$ ). If the global root is down a  $j$ -path adjacent to  $w_2$  (other than  $(w_2, w_4)$ ), then the root of  $F_i$  is on an  $i$ -path adjacent to  $w_1$  (or  $w_1$  itself), and therefore  $F_i$  will release it by Step 1 of the approximation phase. As before,  $F_j$  will release  $w_4$  by Step 3, removing the rest of the contention. A similar argument holds when the global root is down a  $j$ -path adjacent to  $w_4$  (other than  $(w_2, w_4)$ ). If the global root is on  $j$ -path  $(w_2, w_4)$ , or down the  $i$ -path adjacent to  $w_3$  which does not intersect this  $j$ -path, then by Step 1,  $F_j$  releases both  $w_2$  and  $w_4$ , removing all contention.

**Case (3,3,0):** This case cannot arise. By Rule 1 of the forced phase, if it did exist, the branch points of  $F_i$  and  $F_j$  would be interleaved and lie on a path. But then, by applying Rule 3 of the forced phase, we find that at least one of the relevant branch points of  $F_i$  and  $F_j$  would have been claimed during the forced phase.

**Case ( $\alpha > 1, \beta > 1, \gamma > 0$ ):** This case cannot arise after the forced phase, because it requires two branch points of  $F_i$  on a single path of  $F_j$ , which is forbidden by Rule 1 of the forced phase.

**Case ( $3, \beta \leq 1, \gamma$ ):** This case cannot arise after the forced phase, because it requires two branch points of  $F_i$  on a single path of  $F_j$ , which is forbidden by Rule 1 of the forced phase.  $\square$

LEMMA 3.7. *After the approximation phase, every node is in at most one forest  $F_i$ .*

*Proof.* The lemma follows from Lemmas 3.4, 3.5 and 3.6.  $\square$

**4. Approximating Polymorphism. A polymorphic character** (see [13]) allows more than one state per character per species. This type of character has strong application in linguistics [2, 18]. If there are  $r$  states, a polymorphic character is a function  $c : S \rightarrow (2^{\{1, \dots, r\}} - \emptyset)$ , where  $2^{\{1, \dots, r\}}$  denotes the power set (set of all subsets) of  $\{1, \dots, r\}$ . For a given set of species, the *load* is the maximum number of states for any character for any species.

Often the evolution of biological polymorphic characters from parent to child is modelled by mutations, losses and duplications of states between species (see [13]). A **mutation** changes one state into another; a **loss** drops a state from a polymorphic character from parent to child; and a **duplication** replicates a state which subsequently mutates. We associate a cost with each mutation, duplication and loss between a pair of species. In the state-independent model, which we will consider, a loss costs  $c_l$ , a mutation costs  $c_m$  and a duplication costs  $c_d$ , regardless of which states are involved. Following the justification in [2], we insist  $c_l \leq c_m \leq c_d$ . Let  $s_1, s_2 \in S$  and assume  $s_1$  is the parent of  $s_2$ . In the state-independent model, we first look at the differences in cardinality of the parent and child sets. If the parent has fewer states, then we pay the appropriate duplication costs to account for the increased size of the child. If the parent is bigger, then we pay the loss cost. Then we match up as many elements as possible, and pay for the remaining changes as mutations. More specifically, as given in [2], we define  $X = c(s_1) - c(s_2)$ , and  $Y = c(s_2) - c(s_1)$ . Then the cost for the character  $c$  from  $s_1$  to  $s_2$  is  $c_m * |X|$  if  $|X| = |Y|$ , and is  $c_l * [|X| - |Y|] + c_m * |Y|$  if  $|X| > |Y|$  and is  $c_d * [|Y| - |X|] + c_m * |X|$  if  $|Y| > |X|$ .

As input we are given a fixed-topology  $T$  which has a unique species from  $S$  associated with each of its leaves, and label the leaf associated with  $s \in S$  with the set of states  $c(s)$ . The **parsimony problem** is the problem of extending the

function  $c$  to the internal nodes of  $T$  so that the sum of the costs over all edges of  $T$  is minimized. In the monomorphic case (one state per character per species), as discussed earlier, this problem can be solved in polynomial time [7], though the problem of finding a minimum cost labelling is NP-hard if the input does not include a topology [4, 5, 8, 17]. We will consider the **load problem**, introduced in [2]; calculate a labelling of the internal nodes of a fixed topology  $T$  with load at most  $\ell$  and cost at most  $p$ . This problem was shown to be NP-hard in [2], even when  $c_l = 0$  and the topology  $T$  is a binary tree. Note that the dynamic programming techniques presented in Jiang, Lawler and Wang's [11] and Gusfield and Wang's [15] papers do not appear to generalize for the polymorphic load problem. An  $(\alpha, \beta)$ -approximation algorithm for the load problem computes a phylogeny with load at most  $\alpha\ell$  and cost at most  $\beta c$  provided there is a load- $\ell$  cost- $c$  phylogeny. Note that this is a pseudoapproximation algorithm, since the cost of the best  $\alpha\ell$ -load phylogeny may be significantly lower than the cost of the best  $\ell$ -load phylogeny. In this section of the paper, we consider the load problem when  $c_l = 0$  and the topology is arbitrary. We extend the results of section 2 to obtain, for any  $\alpha > 1$ , an  $(\alpha, \frac{\alpha}{\alpha-1})$ -approximation algorithm for the problem. (Note that taking  $\alpha = 2$  gives a  $(2, 2)$ -approximation algorithm.)

We first quote the following observation, which was first noted in [2]:

**OBSERVATION 4.1.** *If  $c_l = 0$ , then if there is a labelling for the topology  $T$  which has load  $\ell$  and cost  $p$ , then there is also a labelling for  $T$  with load  $\ell$  and cost  $p$  such that each internal node contains all the states in the subtree rooted at it or else has load  $\ell$ .*

Therefore to approximate the load we only need to consider the labellings where each internal node contains all the states in the subtree rooted at it or else has load  $\ell$ . We begin by presenting an ILP which provides an exact solution for the load problem. We then use the solution to the linear-programming relaxation of this ILP to compute an  $(\alpha, \frac{\alpha}{\alpha-1})$ -approximation for the problem. The integer program  $\mathcal{P}$  uses the variables  $X_{v,i}$ , for each node  $v$  of the fixed-topology  $T$  and each state  $i \in \{1, \dots, r\}$ , cost variables  $cost_{e,i}$  for each edge  $e \in E(T)$  and each state  $i \in \{1, \dots, r\}$  and the total cost variable  $cost_e$  for each edge  $e$ . These variables have the following interpretation:

$$\begin{aligned} X_{v,i} &= \begin{cases} 1 & \text{if state } i \text{ is in } c(v) \\ 0 & \text{otherwise} \end{cases} \\ cost_{e,i} &= \begin{cases} 1 & \text{if } i \in c(v) \text{ and } i \notin c(u), \text{ for } e = (u \rightarrow v) \\ 0 & \text{otherwise} \end{cases} \\ cost_e &= \sum_{i=1}^r cost_{e,i} \end{aligned}$$

The ILP  $\mathcal{P}$  is then defined as:

minimize  $p$

subject to

$$\begin{aligned} (9) \quad X_{v,i} &= 1 && \text{for each leaf } v \in V(T), \forall i \in c(v) \\ (10) \quad \sum_{i=1}^r X_{v,i} &\leq \ell && \forall v \in V(T) \\ (11) \quad cost_{e,i} &\geq 0 && \forall e \in E(T), i = 1, \dots, r \end{aligned}$$

$$(12) \quad \text{cost}_{e,i} \geq X_{v,i} - X_{u,i} \quad \forall e = (u \rightarrow v) \in E(T), i = 1, \dots, r$$

$$(13) \quad \text{cost}_e = \sum_{i=1}^r \text{cost}_{e,i} \quad \forall e = (u \rightarrow v) \in E(T)$$

$$(14) \quad \sum_{e \in E(T)} \text{cost}_e \leq p/c_m$$

$$(15) \quad X_{v,i}, \text{cost}_{e,i} \in \{0, 1\}$$

The integer program  $\mathcal{P}$  solves the load problem. However, we require only that it provides a lower bound on the best cost. We now show that when we solve  $\mathcal{P}$  with parameter  $\ell$ , the optimal value of  $p$  is a lower bound on the cost of the best load- $\ell$  solution to the fixed topology problem.

LEMMA 4.2. *Let  $S$  be a species set,  $T$  be a fixed topology and  $c : S \rightarrow (2^{\{1, \dots, r\}} - \emptyset)$  be a polymorphic character on  $S$ . If the internal nodes  $v$  of  $T$  can be labelled with subsets of  $\{1, \dots, r\}$  to create a phylogeny for  $c$  with load  $\ell$  and cost  $p$ , then there is a feasible solution for the linear program for this value of  $\ell$  and  $p$ .*

*Proof.* Because of Observation 4.1, we can assume that in the load- $\ell$ , cost- $c$  phylogeny, for each internal node  $v$  in  $V(T)$ , either  $c(v') \subset c(v)$  for every child  $v'$  of  $v$ , or else  $|c(v)| = \ell$ . Therefore the cost of this phylogeny is  $\sum_{(u \rightarrow v) \in E(T)} (c_m * |c(v) - c(u)|) = p$ . Assign values to the  $X_{v,i}$  variable for each internal node  $v$  and to the  $\text{cost}_{e,i}$  variable for each edge  $e = (u \rightarrow v)$  as follows:

$$\begin{aligned} X_{v,i} &= \begin{cases} 1 & \text{if } i \in c(v) \\ 0 & \text{otherwise} \end{cases} \\ \text{cost}_{e,i} &= \begin{cases} 1 & \text{if } i \in c(v) - c(u) \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

This assignment satisfies constraints (15), (10), (11) and (12) of  $\mathcal{P}$ . Constraint (9) is automatically satisfied, and constraint (13) is definitional. Also,  $c_m * \text{cost}_e = c_m * |c(v) - c(u)|$  for every  $e = (u \rightarrow v)$  by definition of the  $\text{cost}_{e,i}$ , and therefore  $\sum_{e \in E(T)} c_m * \text{cost}_e = p$ , and constraint (14) is satisfied.  $\square$

Once again, since integer linear programming is  $\mathcal{NP}$ -hard, we solve the linear-programming relaxation  $\mathcal{LP}$  of  $\mathcal{P}$ , which consists of all the constraints of  $\mathcal{P}$  except that Constraint 15 is replaced with the constraint  $0 \leq X_{v,i}, \text{cost}_{e,i} \leq 1$  (15').

THEOREM 4.3. *Suppose there is a solution for the linear program  $\mathcal{LP}$ . Then we can assign states to the internal nodes of input tree  $T$  such that the resulting phylogeny for  $c$  has load  $\alpha\ell$  and cost no more than  $\left(\frac{\alpha}{\alpha-1}\right)p$ .*

*Proof.* We assign states to the internal nodes of the fixed topology from the leaves upwards. For each internal node  $v \in V(T) - L(T)$ , consider the set  $R(v) = \cup_{(v \rightarrow v') \in E(T)} c(v')$ . If  $|R(v)| \leq \alpha\ell$ , then define  $c(v) = R(v)$ . If  $|R(v)| > \alpha\ell$  then choose the  $\alpha\ell$  states  $i$  of  $R(v)$  which have the greatest  $X_{v,i}$  values. By definition, this assignment of states to the internal nodes of  $T$  has load at most  $\alpha\ell$ .

To show that the cost of this assignment is no more than  $\left(\frac{\alpha}{\alpha-1}\right)p$ , note that the cost on an edge  $e = (u \rightarrow v) \in E(T)$  is  $c_m * |c(v) - c(u)|$ , as  $|c(v) - c(u)|$  is the number of mutations on  $e$ . Our assignment guarantees that if  $|c(u)| < \alpha\ell$  then  $c(u) \supset c(v)$ , which implies  $c_m * |c(v) - c(u)| = 0$ , so we need only consider edges whose upper endpoint has full load. Suppose  $|c(u)| = \alpha\ell$  and  $i \in c(v) - c(u)$ . Then,



by construction of the phylogeny, there is a downwards path from  $v$  to some leaf  $w$  which has  $i \in c(v')$  at every node along the path, including  $w$ . Suppose this path is  $e_1 = (v \rightarrow v_1)$ ,  $e_2 = (v_1 \rightarrow v_2)$ , ...,  $e_j = (v_{j-1} \rightarrow w)$ . By the constraints of the linear program,  $cost_{e,i} + cost_{e_1,i} + \dots + cost_{e_j,i} \geq (X_{v,i} - X_{u,i}) + (X_{v_1,i} - X_{v,i}) + \dots + (X_{w,i} - X_{v_{j-1},i}) = X_{w,i} - X_{u,i}$ , and as  $w$  is a leaf and  $i \in c(w)$ , this is  $1 - X_{u,i}$ . Then, since  $i \notin c(u)$ , and the  $\alpha\ell$  states in  $c(u)$  were chosen to have the greatest  $X_{u,j}$  values, we know  $X_{u,i} \leq \ell/(\alpha\ell + 1)$ . The worst case is achieved when there are  $\alpha\ell + 1$  positive  $X_{u,j}$  values all equal. They sum to at most  $\ell$  from constraint 10, and therefore the smallest one, which cannot be included in the set, has value at most  $\ell/(\alpha\ell + 1)$ . Therefore  $cost_{e,i} + cost_{e_1,i} + \dots + cost_{e_j,i} \geq ((\alpha - 1)\ell + 1)/(\alpha\ell + 1)$ . Furthermore, the costs  $cost_{e,i}, cost_{e_1,i}, \dots, cost_{e_j,i}$  will not be allocated to any other mutation to  $i$ , because any mutation occurring above  $u$  will not have an unbroken path in  $i$  intersecting with any of the edges  $e, e_1, \dots, e_j$ . So every mutation along an edge  $e = (u \rightarrow v) \in T$  with  $|c(u)| = \alpha\ell$  contributes at least  $((\alpha - 1)\ell + 1)/(\alpha\ell + 1)$  to the sum  $\sum_{e \in E(T)} cost_e$  in our linear program. Hence  $p/c_m \geq \sum_{e \in E(T)} cost_e \geq \sum_{e=(u \rightarrow v) \in E(T)} |c(v) - c(u)| \left( \frac{(\alpha-1)\ell+1}{\alpha\ell+1} \right)$ , so the cost  $\sum_{e=(u \rightarrow v) \in E(T)} c_m * |c(v) - c(u)| \leq (\alpha/(\alpha - 1)) * p$ .  $\square$

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