Towards a Data Reduction for the Minimum Flip Supertree Problem

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Abstract. In computational phylogenetics, the problem of constructing a supertree of a given set of rooted input trees can be formalized in different ways, to cope with contradictory information in the input. We consider the Minimum Flip Supertree problem, where the input trees are transformed into a 0/1/?-matrix, such that each row represents a taxon, and each column represents an inner node of one of the input trees. Our goal is to find a perfect phylogeny for the input matrix requiring a minimum number of 0/1-flips, that is, corrections of 0/1-entries in the matrix. The problem is known to be NP-complete. Here, we present a parameterized data reduction with polynomial running time. The data reduction guarantees that the reduced instance has a solution if and only if the original instance has a solution. We then make our data reduction parameter-independent by using upper bounds. This allows us to preprocess an instance, and to solve the reduced instance with an arbitrary method. Different from an existing data reduction for the consensus tree problem, our reduction allows us to draw conclusions about certain entries in the matrix. We have implemented and evaluated our data reduction. Unfortunately, we find that the Minimum Flip Supertree problem is also hard in practice: The amount of information that can be derived during data reduction diminishes as instances get more “complicated”, and running times for “complicated” instances quickly become prohibitive. Still, our method offers another route of attack for this relevant phylogenetic problem.

1 Introduction

When studying the relationship and ancestry of current organisms, discovered relations are usually represented as phylogenetic trees, that is, rooted trees where each leaf corresponds to a group of organisms, called taxon, and inner vertices represent hypothetical last common ancestors (or latest common ancestor) of the organisms located at the leaves of its subtree.

Supertree methods assemble phylogenetic trees with non-identical but overlapping taxon sets, into a larger supertree that contains all taxa of every input tree and describes the evolutionary relationship of these taxa [3]. Constructing a supertree is easy if no contradictory information is encoded in the input trees [7,15]. The major problem of supertree methods is dealing with incompatible data in a reasonable way, where it should be understood that incompatible input trees are the rule rather than the exception in phylogenetic supertree analysis.

Matrix representation (MR) supertree methods encode inner vertices of all input trees as partial binary characters in a matrix, which is then analyzed using an optimization
or agreement criterion to yield the supertree. In 1992, Baum [2] and Ragan [17] independently proposed the matrix representation with parsimony (MRP) method as the first matrix representation method, that performs a maximum parsimony analysis on a matrix representation of the input trees. MRP is by far the most widely used supertree method today, and constructed supertrees are of comparatively high quality. The Maximum Parsimony problem is NP-complete [11], and so is the MRP problem.

The matrix representation with flipping (MRF) supertree method also uses a matrix representation of the rooted input trees, with matrix entries ‘0’, ‘1’, and ‘?’ [9]. Utilizing the parsimony principle, MRF seeks the minimum number of “flips” $0 \rightarrow 1$ or $1 \rightarrow 0$ in the input matrix that make the resulting matrix consistent with a phylogenetic tree, where ‘?’-entries can be resolved arbitrarily. Evaluations by Chen et al. [8] indicate that MRF is on par with the “gold standard” MRP, and superior to other approaches for supertree construction. Most supertree methods take rooted trees as input, and so does MRF; but this is not a problem in practice, as in practically all relevant cases, input trees can be rooted by an outgroup.

If all input trees share the same set of taxa, the supertree is called a consensus tree [1]. As for supertrees, we can encode the input trees in a matrix, here with matrix entries ‘0’ and ‘1’. In case there exist no conflicts between the input trees, we can construct the corresponding perfect phylogeny in $\Theta(mn)$ time for $n$ taxa and $m$ characters [13].

To deal with incompatible input trees, the MRF consensus tree problem again seeks the minimum number of flips in the input matrix to reach a perfect phylogeny. This problem is NP-hard [9], but there have been some recent algorithmic results: The problem can be approximated with approximation ratio $2d$ where $d$ is the maximum number of ones in a column [9]. This approximation ratio is obviously prohibitive in practice, but no constant factor approximation is known. On the parameterized side, let $k$ denote the number of flips required to correct the input matrix: Komusiewicz et al. [14] give a problem kernel with $O(k^3)$ vertices for the MRF consensus tree problem, and Böcker et al. [5] present a $O(4.83^k + poly(m, n))$ search tree algorithm.

For the more general MRF supertree problem, there has been less progress: Clearly, the MRF supertree decision problem is NP-complete, as it generalizes the MRF consensus tree problem, and we can check in polynomial time if a given binary matrix $M^*$ is a perfect phylogeny and has distance at most $k$ to our input matrix. We can test whether an MRF supertree instance admits a perfect phylogeny without flipping in time $\tilde{O}(mn)$ [16]. There exist no approximation algorithms or parameterized algorithms in the literature. Chen et al. [8] present a heuristic for MRF supertrees based on branch swapping, and Chimani et al. [10] introduce an Integer Linear Program (ILP) to find exact solutions. Recently, Böcker et al. [6] presented a heuristic top-down algorithm based on the MRF intuition, namely the FlipCut supertree method, which is both swift and accurate in practice.

Our contributions. Here, we present a set of reduction rules that can be applied to an arbitrary instance of the MRF supertree problem, requiring polynomial running time. Our data reduction is parameterized, in the sense that we assume a maximal number of flips $k$ to be given. The data reduction guarantees that the reduced instance has a
solution if and only if the original instance has a solution. We then show how to make the reduction parameter-independent, by using upper and lower bounds. This allows us to preprocess an instance, and to solve the reduced instance with any method, be it an ILP, a search tree algorithm, or a heuristic. Different from [14], our data reduction allows us to draw conclusions about certain entries in the input matrix, whereas the data reduction for MRF consensus trees in [14] only removes certain characters and taxa from the input.

We have implemented and evaluated our data reduction on a set of MRF supertree instances from [8]. Unfortunately, we find that running times become prohibitive when instances become large, or contain many ‘?’s. This agrees with findings in [10], where “complicated” instances could not be processed by the ILP in reasonable running time. Still and all, we believe that the data reduction presented here, can be an important step towards both exact methods and improved heuristics for the MRF supertree problem.

2 Preliminaries

Let $n$ be the number of taxa and $m$ be the number of characters or features. For brevity, we assume that our set of characters equals $\{1, \ldots, m\}$, and that our set of taxa equals $\{1, \ldots, n\}$. Each taxon $t$ can possess or not possess each character $v$, encoded in a binary $n \times m$ matrix $M$, where columns of $M$ correspond to characters and rows correspond to taxa. For the moment, we do not allow ‘?’ to appear in the input matrix. Under the classical perfect phylogeny model [18], we assume that there exists an ancestral species that possesses none of the characters, corresponding to a row of zeros. We further assume that each transition from ‘0’ to ‘1’ happens at most once in the tree: An invented character never disappears and is never invented twice. We say that $M$ admits a perfect phylogeny if there is a rooted tree with $n$ leaves corresponding to the $n$ taxa, where for each character $u$, there is an inner node $w$ of the tree such that $M[t, u] = 1$ holds if and only if taxon $t$ is a leaf of the subtree below $u$, for all $t$.

Given an arbitrary binary matrix $M$, we may ask whether $M$ admits a perfect phylogeny. Gusfield [13] shows how to test $M$ and, if possible, construct the corresponding phylogenetic tree in time $\Theta(mn)$. There exist several characterizations for such matrices [16], of which we only mention two here. Let $I_M(v) := \{t : M[t, v] = 1\}$ be the set of ‘1’-indices in column $v$. Matrices that admit a perfect phylogeny can be characterized via the pairwise compatibility of all column pairs $u, v$: That is, $I_M(u) \subseteq I_M(v)$ or $I_M(v) \subseteq I_M(u)$ or $I_M(u) \cap I_M(v) = \emptyset$ must hold. Characters that do not satisfy this condition are said to be in conflict. We can also characterize such matrices via local conflicts: Let $G(M)$ be the bipartite graph on character vertices $v \in \{1, \ldots, m\}$ and taxa vertices $t \in \{1, \ldots, n\}$, such that an edge $(v, t)$ exists if and only if $M[t, v] = 1$. Now, $M$ admits a perfect phylogeny if and only if the graph $G(M)$ is $M$-free, that is, it does not contain an induced path of length four starting from and ending in different taxa vertices [9].

We consider two variants of Matrix Representation with Flipping problems, namely the Minimum Flip Consensus Tree (MFCT) and the Minimum Flip Supertree (MFST) problem. For the MFCT problem, consider a set of binary rooted trees on the
same set of $n$ taxa. We encode the input trees in a binary matrix $M$, where each column corresponds to an inner node in one of the trees, and an entry ‘1’ indicates that the corresponding taxon is a leaf of the subtree rooted in the inner node. We ask for the minimum number of modifications (“flips”) to $M$ such that the resulting matrix admits a perfect phylogeny. We refer to this number of flips as the cost of the instance.

The more general MFST problem arises when the input trees have overlapping but not necessarily identical taxa sets. In this case, for characters belonging to a particular input tree, the state (‘0’ or ‘1’) of some taxa is not known as they are not part of the input tree, and represented by a question mark (‘?’). We ask for a perfect phylogeny matrix $M^*$ such that the number of entries where one matrix contains a ‘0’ and the other matrix a ‘1’, is minimal. This is the number of flips required to correct the input matrix $M$, whereas ‘?’-entries can be resolved arbitrarily. Note that a perfect phylogeny matrix must not contain ‘?’ entries. Both for MFST and MFCT, we usually have $n \ll m$.

Throughout this paper, we assume that the input matrix $M$ does not contain any all-zero columns: If the matrix would contain such columns, we could simply remove them. We infer that any optimal solution does not contain an all-zero column: Otherwise, we could leave one of the entries in the flipped matrix $M^*$ in its original state ‘1’, thereby constructing a matrix that is also a perfect phylogeny but requires less flipping. This follows because a character that is exhibited by a single taxon, cannot be in conflict with any other character. We make use of the fact throughout this paper without explicitly referring to it.

### 3 The inclusion graph

Given an instance $M \in \{0, 1\}^{n \times m}$ of the Minimum Flip Consensus Tree problem, we say that two characters $u$ and $v$ are in conflict if $I_M(u) \cap I_M(v) \neq \emptyset$ but $I_M(u) \not\subseteq I_M(v)$ and $I_M(v) \not\subseteq I_M(u)$. We define the inclusion graph $G = (V, E)$ as follows: This graph has vertex set $V := \{1, \ldots, m\}$, being the characters of matrix $M$. Two vertices $u, v \in V$ can be connected via a directed edge $(u, v)$, or by an undirected edge $uv = \{u, v\}$. An inclusion edge $(u, v)$ from $u \in V$ to $v \in V$ is present if $I_M(u) \subseteq I_M(v)$. A disjoint edge $uv$ connecting $u, v \in V$ is present if $I_M(u) \cap I_M(v) = \emptyset$. Any two vertices $u, v$ are connected by either no edge in case $u, v$ are in conflict; by a single edge $(u, v)$, $(v, u)$, or $uv$; or, by two inclusion edges $(u, v)$ and $(v, u)$ at the same time.

If two vertices $u, v \in V$ are connected by both directed edges $(u, v)$ and $(v, u)$, then $u$ and $v$ have the same neighborhood $I_M(u) = I_M(v)$. In this case, there exists an optimal solution such that $u$ and $v$ also have the same neighborhood \cite{14}. There may also exist optimal solutions such that $u$ and $v$ have different neighborhoods, but this case is somewhat pathogenic and will rarely appear in practice. In view of this, we can immediately merge $u$ and $v$. In order to merge nodes in the inclusion graph, we assume that each character vertex $v \in V$ and each column of the matrix $M$ has a weight assigned to it, representing its multiplicity. For readability, we omit these simple details in the following. Now, we may assume that any two vertices $u, v \in V$ are connected by at most one edge.
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We know that \( M \) admits a perfect phylogeny if and only if there exist no two vertices \( u, v \in V \) that are in conflict. This is the case if any two vertices in the inclusion graph are connected by (at least) one edge. When resolving conflicts in the matrix \( M \), this will lead to induced changes in the inclusion graph. This allows us to reformulate our problem: We search for the minimum number of changes in \( M \), such that any two vertices in the inclusion graph are connected by (at least) one edge.

If \( M \) admits a perfect phylogeny, then the resulting graph is transitive: from \((u, v) \in E\) and \((v, w) \in E\) we infer \((u, w) \in E\). But we can derive a similar deduction rule for disjoint edges: from \((u, v) \in E\) and \(vw \in E\) we infer \(uw \in E\). We say that an inclusion graph is tree-ish if it satisfies these deduction rules for all vertices.

In applications, it is of no avail to actually compute the inclusion graph of a matrix \( M \), as we can compute on the fly whether an edge is present or not, using \( M \). Still, the inclusion graph is useful in applications: During data reduction, we sometimes learn that, say, \( I_M(u) \subseteq I_M(v) \) must hold for the optimal solution. In this case, we set the respective edge to “permanent”. More often, we will learn from the data that, say, \( I_M(u) \subseteq I_M(v) \) cannot hold for the optimal solution. In this case, we set the respective edge to “forbidden”. Note that forbidden edges may co-exist in parallel for one vertex pair \( u, v \). But in case two out of the three edges \((u, v), (v, u), \) and \(uv\) are set to forbidden, we can immediately set the remaining edge to permanent.

The inclusion graph, in turn, allows us to draw conclusions about entries in \( M \): If there is a permanent edge \((u, v)\) in the inclusion graph, and we decide to change or keep an entry \( M[t, u] = 1 \) in our input matrix, this forces us to also set \( M[t, v] = 1 \). Similarly, if we decide to change or keep an entry \( M[t, v] = 0 \) then the edge \((u, v)\) in the inclusion graph also forces us to set \( M[t, u] = 0 \). We will formalize these observations in the next section.

Note that we can define a similar inclusion graph for an instance \( M \in \{0, 1, ?\}^{n \times m} \) of the Minimum Flip Supertree problem. Here, \( M \) admitting a perfect phylogeny \( M^* \) does not imply that every two vertices in the inclusion graph are connected by an edge: For example, an input matrix containing solely ‘?’ results in an inclusion graph without edges. But our other reasoning introduced above, remains valid.

4 Parameterized data reduction

We now describe data reduction rules for the Minimum Flip Supertree problem. Here, entries in the matrix \( M \) can be ‘?’ and we have to assure that such entries are chosen “conservatively”: To this end, we define \( I_M^*(v) := \{ t : M[t, v] \in \{1, ?\} \} \).

We take a parameterized view of the problem: We assume that we are given an integer \( k \), and we want to know if there exists a solution for input matrix \( M \) with cost at most \( k \). This will allow us to set certain edges of the inclusion graph to forbidden or permanent, and also to permanently set certain entries in the matrix \( M \), which may include resolving ‘?’-entries or even flipping entries in the matrix. We will see in Sec. [5] how these rules can be applied during preprocessing.

For \( u, v \in V \) we set \( N(u - v) := I_M(u) \setminus I_M^*(v) \) and \( N(u + v) := I_M(u) \cap I_M(v) \). Recall that \((u, v)\) being present in the inclusion graph of an optimal solution \( M^* \in \)
\{0, 1\}^{n \times m}$, implies that $I_M^*(u) \subseteq I_M^*(v)$ must hold. Similarly, $uv$ being present implies that $I_M^*(u) \cap I_M^*(v) = \emptyset$. As we assume that the distance between $M^*$ and $M$ is at most $k$ flips, we can easily deduce two simple reduction rules:

**Rule 1.** If $|N(u - v)| > k$ then set $(u, v)$ to forbidden.

**Rule 2.** If $|N(u + v)| > k$ then set $uv$ to forbidden.

Note that the first rule is two-sided, as edges $(u, v)$ are directed. In case two of the three possible edges $(u, v), uv, (v, u)$ between vertices $u, v$ have been set to forbidden, we set the remaining edge to permanent. If an edge is set to permanent and forbidden simultaneously or, equivalently, if all three edges $(u, v), uv, (v, u)$ are set to forbidden simultaneously, then the instance has no solution with cost at most $k$. In case entries in $M$ have been permanently set, we can extend these rules as follows: We assume $|N(u - v)| = \infty$ if both $M[t, u] = 1$ and $M[t, v] = 0$ are permanent for some taxon $t$; and $|N(u + v)| = \infty$ if both $M[t, u] = 1$ and $M[t, v] = 1$ are permanent for some taxon $t$.

On the other hand, we can use permanent edges in $G$ to derive information about entries in $M$: Keeping or setting some entry $M[t, u]$, will require us to also change other entries in $M$. The next three rules follow immediately:

**Rule 3.** If $M[t, u] = 1$ is permanent and $(u, v)$ is permanent in $G$, then permanently set $M[t, v] = 1$.

**Rule 4.** If $M[t, v] = 0$ is permanent and $(u, v)$ is permanent in $G$, then permanently set $M[t, v] = 0$.

**Rule 5.** If $M[t, u] = 1$ is permanent and $uv$ is permanent in $G$, then permanently set $M[t, v] = 0$.

Again, if an entry $M[t, u]$ is permanently set to ‘0’ and ‘1’ simultaneously, then the instance has no solution with cost at most $k$.

Based on these observations, we can test in advance if the instance still allows to permanently set an entry of the matrix to ‘0’ or ‘1’. The **induced cost one** for entry $M[t, u]$, denoted $ico(t, u)$, is the number of vertices $v \in V$ such that $(u, v)$ is permanent and $M[t, v] = 0$, plus the number of vertices $w \in V$ such that $uv$ is permanent and $M[t, w] = 1$. Similarly, we define the **induced cost zero** for entry $M[t, v]$, denoted $icz(t, v)$, as the number of vertices $u \in V$ such that $(u, v)$ is permanent and $M[t, u] = 1$. We also take into account if the entry $M[t, v]$ is currently set to ‘0’, ‘1’, or ‘?’.

To this end, we define $ico_*(t, u) := ico(t, u) + 1$ if $M[t, u] = 0$, and $ico_*(t, u) := ico(t, u)$ otherwise. Similarly, we define $icz_*(t, v) := icz(t, v) + 1$ if $M[t, v] = 1$, and $icz_*(t, v) := icz(t, v)$ otherwise.

**Rule 6.** If $ico_*(t, u) > k$ then permanently set $M[t, u] = 0$.

**Rule 7.** If $icz_*(t, v) > k$ then permanently set $M[t, v] = 1$.

We can do the inverse reasoning of Rules 6 and 7 and reach:

**Rule 8.** If $M[t, u] = 1$ is permanent and $M[t, v] = 0$ is permanent then set $(u, v)$ to forbidden.
Rule 9. If $M[t,u] = 1$ is permanent and $M[t,v] = 1$ is permanent then set $uv$ to forbidden.

Finally, we can use the fact that the inclusion graph must be tree-ish:

Rule 10. If $(u,v)$ is permanent and $(v,w)$ is permanent then set $(u,w)$ to permanent.
Rule 11. If $(u,v)$ is permanent but $(u,w)$ is forbidden then set $(v,w)$ to forbidden.
Rule 12. If $(v,w)$ is permanent but $(u,w)$ is forbidden then set $(u,v)$ to forbidden.
Rule 13. If $(u,v)$ is permanent and $vw$ is permanent then set $uw$ to permanent.
Rule 14. If $(u,v)$ is permanent but $uw$ is forbidden then set $vw$ to forbidden.
Rule 15. If $vw$ is permanent but $uw$ is forbidden then set $(u,v)$ to forbidden.

Finally, we can get rid of characters exhibited by a single taxon:

Rule 16. If a column in $M$ contains at most one ‘1’ entry, then remove this column.

Given an instance of MFST, we apply the above data reduction rules until the conditions of none of the rules are met. Whenever we change an entry of the matrix $M$ by the above rules, we can lower our parameter $k$ by one which, in turn, may allow us to apply other rules. Still, the complete data reduction requires only cubic time:

Theorem 1. Rules 1–16 are correct, and can be carried out to completion in $O((m + n)m^2)$ time.

Proof. From the reasoning above, it is quite obvious that all rules are correct. So, we focus on the running time of the data reduction.

Given an instance $M$ of the MFST problem, we first compute the inclusion graph in time $O(m^2n)$. Note that in the matrix $M$, at most $O(mn)$ entries can be permanently set to ‘0’ or ‘1’ during the course of the data reduction. Similarly, at most $O(m^2)$ edges can be set to forbidden or permanent in the inclusion graph. Whenever we permanently flip an entry in $M$, we lower our cost bound $k$ by one.

Initially, we compute $q(u-v) := |N(u-v)|$ and $q(u+v) := |N(u+v)|$ for all $u,v$ in time $O(m^2n)$. Now, we can test Rules 1–2 in constant times for each pair $u,v$. Similarly, we compute $ico_s(t,v)$ and $icz_s(t,v)$ for all $v,t$ in time $O(m^2n)$, what allows us to test Rules 6–7 in constant time for each pair $t,v$. During the course of our data reduction, the parameter $k$ will change, so we have to efficiently find those pairs $u,v$ or $t,v$ that allow to use one of these rules. For each value $0, \ldots, k$ as well as all values $> k$ we use an individual bin, and we use double-linked lists to access those pairs that allow application of the above rules. Updating $q(u-v)$, $q(u+v)$, $ico_s(t,v)$, and $icz_s(t,v)$ can still be performed in constant time. So, in constant time we can find a pair $u,v$ or $t,v$ to apply a reduction rule, or decide that no such pair exists.

All other rules are only applied if a matrix entry is permanently set or flipped, or if an edge in the inclusion graph is set to forbidden or permanent. For each rule, we now analyze under what circumstances it can be applied, an what time is required to apply the rule.

For Rules 1–4 we have to update $q(u-v)$ and $q(u+v)$ every time an entry in the matrix is flipped. Assume that $M[t,u]$ is the matrix entry being flipped, then we check
for all \( v \neq u \), whether \( q(u - v) \), \( q(v - u) \), or \( q(u + v) \) must be updated. In this case, these values are increased or decreased by one, depending on the entry \( M[t, v] \). In total, a flip in the matrix \( M \) requires \( O(m) \) time to update all \( q(u - v) \) and \( q(u + v) \).

Rules [8][9] must be applied if either a matrix entry is permanently set, or if an edge is set to forbidden or permanent. Regarding Rule [8], assume that \( M[t, u] \) is permanently set to ‘1’. In this case, we have to test for all \( v \neq u \) if \( (u, v) \) is permanent in the inclusion graphs, what can be done in time \( O(m) \). Now, assume that some edge \( (u, v) \) is set to permanent. Then, we have to check all taxa \( t \) if \( M[t, u] = 1 \) is permanent, what can be done in time \( O(n) \). A similar reasoning applies for the other two rules.

Rules [8][9] require us to update \( ico_s(t, v) \) and \( icz_s(t, u) \) whenever either a matrix entry is flipped, or an edge is set to permanent. Regarding \( ico_s(\cdot) \), assume that entry \( M[t, v] \) has been flipped to ‘0’. Then, for all \( u \neq v \) such that \( (u, v) \) is permanent, we increase \( ico_s(t, u) \) by one. Similarly, for all \( u \neq v \) such that \( uvw \) is permanent, we decrease \( ico_s(t, w) \) by one. If \( M[t, v] \) has been flipped to ‘1’ then we do the same, exchanging increase and decrease. This can be carried out in time \( O(m) \). If an edge is set to permanent, we can update all affected entries in time \( O(n) \). A similar reasoning applies for the computation of \( icz_s(t, u) \).

For Rules [8][9] we have to update edges in case an entry \( M[t, v] \) is flipped: Then, we have to consider all entries \( M[t, u] \) for \( u \neq v \) what can be done in time \( O(m) \).

Rules [10][15] update edges in case some edge between \( u \) and \( v \) is set to forbidden or permanent: Then, we have to consider all vertices \( w \neq u, v \) what requires \( O(m) \) time.

Applying the above rules, may result in more than one “update operations” to be carried out. For that, we can keep all such update operations on a stack, and carry out the next update operation only after we have finished the current one.

We conclude that permanently setting an entry of the matrix requires \( O(m) \) time for checking all of the rules. Since we can permanently set at most \( O(mn) \) entries, this requires \( O(m^2n) \) time in total. Similarly, setting an edge to permanent, requires \( O(m + n) \) time for checking our rules. Since there are \( O(m^2) \) edges the total running time becomes \( O((m + n)m^2) \). This results in a running time of \( O((m + n)m^2) \) for the full data reduction. \( \square \)

If we reach a conflict in our data reduction, such as permanently setting some \( M[t, v] \) to 0 and 1 at the same time, then we infer that there exists no solution of the instance of cost at most \( k \).

5 Upper and lower bounds

We will now describe a lower bound for the minimum flip supertree problem, which we will use to derived improved versions of Rules [1][2] and [6][7]. A local conflict consists of two characters \( u, v \in \{1, \ldots, m\} \) and three taxa \( t_1, t_2, t_3 \in \{1, \ldots, n\} \) such that \( M[t_1, u] = M[t_2, v] = M[t_3, v] = 1 \) but \( M[t_3, u] = M[t_1, v] = 0 \). In the minimum flip consensus tree setting, \( M \) admits a perfect phylogeny if and only if \( M \) does not contain a local conflict [9]. For MFST, we can only reason that if \( M \) contains a local conflict, then it does not admit a perfect phylogeny.
We now use local conflicts to compute a lower bound for the costs of an instance $M$: We say that two local conflicts are edge-disjoint if the local conflicts do not contain a common tuple $(v, t)$. The term “edge-disjoint” stems from visualizing the matrix $M$ as a bipartite graph $[9]$, as noted in Sec. 2. Let $C$ be a set of edge-disjoint local conflicts in $M$. Now, for every element in $C$ we have to make at least one modification to the matrix $M$ to remove the local conflict, so $|C|$ is a lower bound to the cost of an optimal solution. Unfortunately, it is not obvious how to efficiently find a set $C$ of maximal cardinality: For example, the obvious transformation to a graph leads to the NP-hard MAXIMUM INDEPENDENT SET problem. In case columns of $M$ have been weighted, we can follow a greedy strategy, choosing a local conflict that maximizes the cost of the current step. We can also weight each local conflict by the (inverse) number of other local conflicts it has at least one common edge with. Finally, we can restart the algorithm several times, choosing a random local conflict in each step, and maximize over these bounds. In theory, we can compute another lower bound by solving the relaxation of the Integer Linear Program presented in [10], but this is usually too slow in practice.

Testing all characters $u, v$ and taxa $t_1, t_2, t_3$ is prohibitive in application, as this requires $O(m^2 n^3)$ time. But we can use sets $N(u - v)$ and $N(u + v)$ for this purpose: Two characters are in conflict if all sets $N(u - v), N(u + v), N(v - u)$ contain at least one element. We now describe an improved algorithm for the greedy strategy and its variants discussed above. Initially, we compute the cardinality $q(u - v)$ and $q(u + v)$ in $O(m^2 n)$ time, storing $q$ requires $O(m^2)$ space. We start with a set $L = \{ (u, v) : 1 \leq u < v \leq m \}$ of character pairs that are potentially in conflict. We then select a pair $(u, v)$ from $L$, either randomly or by some other criterion. If $u, v$ are no longer in conflict, we remove $(u, v)$. Otherwise, we choose a certain local conflict $u, v, t_1, t_2, t_3$ to be part of our set $C$. We then update, for each tuple $(w, t)$ of the local conflict, $w \in \{ u, v \}$ and $t \in \{ t_1, t_2, t_3 \}$, all cardinalities $q(w - w')$, $q(w + w')$, and $q(w' - w)$ for all characters $w'$ in time $O(mn)$. Let $k_{opt}$ be the cost of an optimal solution, then $|C| \leq k_{opt} \leq mn$. All updates require $O(|C| mn)$ time and, hence, $O(k_{opt} mn)$ time. The whole procedure requires only $O(k_{opt} mn + m^2 n)$ time in total. In practice, we can speed up calculations by initializing $L$ with those tuples $(u, v)$ that are initially in conflict. Also, note that our data reduction requires us to maintain cardinalities $q$ before we enter the computation of a lower bound.

We now use a trick introduced in [4] to lift a local reduction rule to a global version: Rules 1–2 are local, in the sense that these rules only take into account entries $M[t, u]$ and $M[t, v]$ for all taxa $t$. Similarly, computing $ico_*(t, v)$ and $icz_*(t, v)$ will consider entries $M[t, w]$ for all characters $w$, but ignore the rest of the matrix. As all other rows or columns of $M$ have to be cleaned of local conflicts at a later stage, it makes sense to estimate the cost for doing so using a lower bound.

Let $lb_M(t)$ be any lower bound where, during the calculation of this bound, the row of $M$ corresponding to taxon $t$ is not taken into account. Similarly, we write $lb_M(u, v)$ for two ignored character columns $u, v$. Now, we can write improved versions of Rules 1–2 and 6–7.

**Rule 17.** If $|N(u - v)| + lb_M(u, v) > k$ then set $(u, v)$ to forbidden.
Rule 18. If $|N(u + v)| + lBM(u, v) > k$ then set $uv$ to forbidden.
Rule 19. If $ico_s(t, v) + lBM(t) > k$ then permanently set $M[t, v] = 0$.
Rule 20. If $icz_s(t, u) + lBM(t) > k$ then permanently set $M[t, u] = 1$.

The correctness of these rules follows immediately. Unfortunately, we have to compute an individual lower bound $lBM(u, v)$ for every pair $u, v$ and $lBM(t)$ for every $t$. To further speed up calculations, we can initially compute a lower bound $lbM$ of the complete instance, and calculate $lbM(u, v)$ only for those pairs where $|N(u - v)| + lBM > k$ or $|N(u + v)| + lBM > k$ holds. Note that there may exist rare cases where our lower bound computations are not monotonous, so that $lbM(u, v) > lBM$, and we will miss a rule that could have been applied. We expect this to be negligible in practice. A similar reasoning applies for $lBM(t)$.

The above rules still depend on parameter $k$. To reach a parameter-independent data reduction, we have to choose an appropriate $k$: To this end, note that the cost of any heuristic solution to an instance, are always an upper bound to the cost of an optimal solution. So, we can choose any heuristic to compute an appropriate $k$, and then apply our parameter dependent data reduction, using a lower bound for Rules 17–20. It must be understood that for practically all real-world instances, the cost $k$ computed by any heuristic will be too large to directly apply Rules 1–2 and 6–7. Only through our algorithm engineering technique of using lower bounds, we can successfully start our data reduction. Rules 19 and 20 will sometimes allow us to lower the cost $k$ and, hence, the complexity of the remaining instance.

Chen et al. [8] have introduced an involved heuristic for the problem that, much like heuristics for the Maximum Parsimony problem, is based on exploring tree space via branch swapping. This heuristic is rather time-consuming and can require minutes or even hours of running time, but its results are of excellent quality [10]. Another upper bound can be computed by running the ILP from [10] for some time, and stop after a fixed time before upper and lower bound of the instance coincide.

6 Experiments

We implemented all evaluated algorithms in Java. Computations were performed on an AMD Opteron-275 2.2 GHz with 6 GB of memory running Solaris 10.

We now evaluate the parameter-independent data reduction. As indicated in the introduction, we can use our reduction as a preprocessing step, and solve the reduced instance with any exact, approximation, or heuristic algorithm. To evaluate the performance of our data reduction, we use different measures:

- We calculate the ratio of fixed entries, ‘0/1’ entries that are not flipped by the data reduction but set to permanent, relative to the number of ‘0/1’ entries in the input matrix.
- Similarly, we calculate the ratio of flipped entries, which are always permanent.
- We calculate the ratio of resolved entries, ‘?’ entries that are permanently set to ‘0/1’, relative to the number of ‘?’ entries in the input matrix.
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| Taxa $n$ | 48 | 48 | 48 | 96 |
|----------|----|----|----|----|
| Input trees $s$ | 4  | 6  | 8  | 4  |
| Fixed entries | 36.13 | 30.43 | 24.64 | 7.46 |
| Flipped entries | 0.04 | 0.04 | 0.04 | 0.002 |
| Resolved entries | 31.90 | 28.69 | 23.69 | 6.23 |
| Permanent entries | 35.12 | 30.03 | 24.43 | 7.26 |
| Permanent edges | 29.28 | 25.46 | 20.20 | 4.92 |
| Forbidden edges | 28.22 | 23.63 | 19.03 | 7.68 |
| Number flips | 2.02 | 3.07 | 3.51 | 0.51 |
| No. flips relative | 12.26 | 9.88 | 8.78 | 1.11 |
| Running time (h:min) | 0:50 | 5:40 | 22:51 | 24:08 |

Table 1. Results of the data reduction for 25% taxa deletion. Averages over 100 instances. All numbers except “number flips” and “running time” in percent.

- We calculate the ratio of permanent entries in the matrix, relative to the size $mn$ of the matrix.
- Next, we count how many edges in the inclusion graph have been set to permanent, and compare this to the $\binom{m}{2}$ possible edges.
- For all pairs $u, v$ where no permanent edge exists, we count the number of forbidden edges, and compare this to the $3\binom{m}{2}$ possible forbidden edges.
- Finally, we calculate the number of flips executed by the data reduction, and compare it to the number of flips required to solve the instance. This reduces the cost and, hence, the complexity of the resulting instance.

For our evaluation, we use instances generated by Eulenstein et al. [12], see there for details. These simulated datasets are very similar to a regular phylogenetic supertree study, yet for each dataset we know the true model tree behind the data. Unfortunately, running times of our data reduction are currently prohibitive for larger instances as well as instances with a large fraction of ‘?’. To this end, we concentrate on matrices containing 25% ‘?’-entries, generated from $s = 4, 6, 8$ input trees. The number of taxa $n$ is either 48 or 96. These matrices contain about $m \approx (pn - 2)s$ columns, where $1 - p$ is the ratio of ‘?’-entries. For each parameter combination, we choose the 100 instances named “random”, for which deleted taxa were randomly chosen. We use the heuristic solutions from [8] as upper bounds for our parameter-independent data reduction, and the randomized lower bound from Sec. 5 with 100 repetitions.

One can see that reduction ratios deteriorate for both increasing number of input trees, and increasing number of taxa. We expect this to be even more so for higher ratios of taxa deletion. Currently, the limiting factor are the high running times of the data reduction. On the other hand, we observe that the data reduction truly does reduce the instances. This is a clear indication that with an improved implementation, algorithm engineering, new data reduction rules, and an improved lower bound, we may indeed simplify MFST instances in polynomial time.
We have presented a set of data reduction rules, that allow us preprocess instances of the Minimum Flip Supertree problem, and also of the “simpler” Minimum Flip Consensus Tree problem. Our data reduction can be applied in polynomial running time. Different from [14], our reduction allows us to draw conclusions about certain entries in the input matrix. This is highly desirable, as flipping entries during preprocessing means that we are reducing the cost of the resulting instance: Chimani et al. [10] found that ILP running times are strongly correlated with the optimal number of flips.

Our method allows us to draw conclusions about MFST instances, guaranteeing both polynomial running time and optimality of the solution. On the practical side, the output of our method can be subsequently processed with any method, including fast heuristics. Unfortunately, our reduction is currently not suited for real-world application, as running times are prohibitive and reduction results are minor. Still, we think that this an important first step towards a data reduction that is applicable in practice. An improved data reduction may be ultimately combined with heuristics to obtain a supertree method that is both fast and accurate in practice.

Note that the inclusion graph can also be used as an algorithm engineering technique for the MFCT search tree algorithm from [5]. We conjecture that these techniques will make the search tree algorithm much faster in practice. Unfortunately, it appears this cannot be used to improve upon the worst-case running time of the algorithm.

We conjecture that our data reduction from Sec. 4 can be used as part of a problem kernel for the MFCT problem. From the theoretical side, it is an interesting open question if this allows us to find a better than cubic kernel [14]. Finding a kernel for the MFST problem, on the other hand, is related to the open question whether MFST is parameterized tractable.

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